HUMBOLDT-UNIVERSITÄT ZU BERLIN
MATHEMATISCH-NATURWISSENSCHAFTLICHE FAKULTÄT
INSTITUT FÜR MATHEMATIK

Optimal control of a semi-discrete Cahn–Hilliard–Navier–Stokes system with variable fluid densities

Dissertation

zur Erlangung des akademischen Grades

doctor rerum naturalium

(Dr. rer. nat.)

im Fach Mathematik

eingereicht an der
Mathematisch-Naturwissenschaftlichen Fakultät
der Humboldt-Universität zu Berlin

von
Dipl.-Math. Tobias Keil

verteidigt am 10.09.2021

Präsidentin der Humboldt-Universität zu Berlin
Prof. Dr.-Ing. Dr. Sabine Kunst

Dekan der Mathematisch-Naturwissenschaftlichen Fakultät
Prof. Dr. Elmar Kulke

Gutachter: Prof. Dr. Michael Hintermüller
Prof. Dr. Charles M. Elliott
Prof. Dr. Michael Hinze

Abstract

This thesis is concerned with the optimal control of a time-discrete Cahn–Hilliard–Navier–Stokes system with variable fluid densities. It focuses on the double-obstacle potential, which yields an optimal control problem for a family of coupled systems in each time instant of a variational inequality of fourth order and the Navier–Stokes equation. A suitable time-discretization is presented and associated energy estimates are proven. The existence of solutions to the primal system and of optimal controls is established for the original problem as well as for a family of regularized problems. The latter correspond to Moreau–Yosida type approximations of the double-obstacle potential. The consistency of these approximations is shown and first order optimality conditions for the regularized problems are derived. Through a limit process with respect to the regularization parameter, a stationarity system for the original problem is established. The resulting system corresponds to a function space version of ε-almost C-stationarity, which is a special notion of stationarity for MPECs.

Moreover, a numerical solution algorithm for the optimal control problem is developed based on a penalization method involving the Moreau–Yosida type approximations of the double-obstacle potential. A dual-weighted residual approach for goal-oriented adaptive finite elements is presented which is based on the concept of C-stationarity. The overall error representation depends on primal residuals weighted by approximate dual quantities and vice versa, supplemented by additional terms corresponding to the complementarity mismatch. The numerical realization of the adaptive concept is described and a report on numerical tests is provided.

The Lipschitz continuity of the control-to-state operator of the corresponding instantaneous control problem is verified and its directional derivative is characterized by a system of variational inequalities and partial differential equations. Strong stationarity conditions for the instantaneous control problem are derived based on a technique pioneered by Mignot and Puel. Utilizing the primal notion of B-differentiability, a bundle-free implicit programming method is developed. Details on the numerical implementation are given and numerical results for representative examples are included.

Zusammenfassung

Die vorliegende Doktorarbeit befasst sich mit der optimalen Steuerung von semidiskreten Cahn–Hilliard–Navier–Stokes-Systemen mit unterschiedlichen Flüssigkeitsdichten. Dabei konzentriert sie sich auf das Doppelhindernispotential, was zu einem optimalen Steuerungsproblem einer Gruppe von gekoppelten Systemen, welche zu jedem Zeitschritt eine Variationsungleichung vierter Ordnung sowie eine Navier–Stokes-Gleichung beinhalten, führt. Eine geeignete Zeitdiskretisierung wird präsentiert und zugehörige Energieabschätzungen werden bewiesen. Die Existenz von Lösungen zum primalen System und von optimalen Steuerungen für das ursprüngliche Problem sowie für eine Gruppe von regularisierten Problemen wird etabliert. Die regularisierten Probleme stehen in Zusammenhang mit Moreau–Yosida-artigen Approximationen des Doppelhindernispotentials. Die Konsistenz der Approximierungsmethode wird gezeigt und Optimalitätsbedingungen erster Ordnung für die regularisierten Probleme werden hergeleitet. Mittels eines Grenzübergangs in Bezug auf den Regularisierungsparameter werden Stationaritätsbedingungen für das ursprüngliche Problem etabliert. Diese entsprechen einer Form von C-Stationarität im Funktionenraum, welches eine spezielle Form der Stationarität für mathematische Optimierungsprobleme mit Gleichgewichtsbedingungen ist.

Weiterhin wird ein numerischer Lösungsalgorithmus für das Steuerungsproblem basierend auf einer Strafmethode entwickelt, welche die Moreau–Yosida-artigen Approximationen des Doppelhindernispotentials einschließt. In diesem Zusammenhang wird ein dual-gewichteter Residuenansatz für zielorientierte adaptive finite Elemente präsentiert, welcher auf dem Konzept der C-Stationarität beruht. Der entsprechende Fehlerschätzer hängt von den primalen und dualen Residuen, welche jeweils mit Approximationen der dualen bzw. primalen Größen gewichtet werden, ab. Außerdem enthält er zusätzliche Terme, die die Diskrepanz in der Komplementarität wiederspiegeln. Die numerische Realisierung des adaptiven Konzepts und entsprechende numerische Testergebnisse werden beschrieben.

Die Lipschitzstetigkeit des Steuerungs-Zustandsoperators des zugehörigen instantanen Steuerungsproblems wird bewiesen und dessen Richtungsableitung wird durch ein System von Variationsungleichungen und partiellen Differentialgleichungen charakterisiert. Starke Stationaritätsbedingungen für dieses Problem werden durch die Anwendung einer Technick von Mignot und Puel hergeleitet. Basierend auf der primalen Form der Bouligard-Ableitung wird ein impliziter numerischer Löser entwickelt, dessen Implentierung erläutert und anhand von numerischen Resultaten inllustriert wird.

I would like to thank my family, my friends, my colleagues and, in particular, my supervisor Prof. Dr. Michael Hintermüller for their ongoing support, the inspiring and helpful discussions, and their scientific advice throughout the course of my doctoral studies.

I would also like to thank my colleagues Prof. Dr. M. Hinze, Dr. C. Kahle and Dr. D. Wegner for the fruitful collaborations on the optimal control of multiphase flows, and, in particular, Dr. C. Kahle for sharing his expertise on the numerical realization of adaptive solution algorithms in a C++ environment.

Contents

Introduction

The main subject of this thesis is the optimal control of multiphase flows including two (or more) immiscible fluids. The primary focus is on a coupled system consisting of a Navier–Stokes type equation, which captures the hydrodynamics of the fluids, and the Cahn–Hilliard system. The latter represents a phase field model describing the spinodal decomposition of different phases. It was introduced by Cahn and Hilliard in [44].

A first basic model for immiscible, viscous two-phase flows combining the Cahn–Hilliard system with the Navier–Stokes equation was published by Hohenberg and Halperin in [123]. It is, however, restricted to the case where the two fluids possess nearly identical densities, i.e. matched densities. In this work, the following more recent diffuse interface model for two-phase flows with non-matched densities is studied

$$
\begin{aligned}
\partial_t \varphi + v \nabla \varphi - \operatorname{div}(m(\varphi) \nabla \mu) &= 0, && \text{(1a)}\\
-\Delta \varphi + \partial \Psi_0(\varphi) - \mu - \kappa \varphi &\ni 0, && \text{(1b)}\\
\partial_t(\rho(\varphi) v) + \operatorname{div}(v \otimes \rho(\varphi) v) - \operatorname{div}(2\eta(\varphi)\varepsilon(v)) + \nabla \Pi & \\
+ \operatorname{div}(v \otimes J) - \mu \nabla \varphi &= 0, && \text{(1c)}\\
\operatorname{div} v &= 0, && \text{(1d)}\\
v_{|\partial\Omega} &= 0, && \text{(1e)}\\
\partial_n \varphi_{|\partial\Omega} = \partial_n \mu_{|\partial\Omega} &= 0, && \text{(1f)}\\
(v, \varphi)_{|t=0} &= (v_a, \varphi_a). && \text{(1g)}
\end{aligned}
$$

It was derived by Abels, Garcke and Grün in [6] and holds in the space-time cylinder $\Omega \times (0, \infty)$, where $\partial\Omega$ denotes the boundary of Ω. The model is thermodynamically consistent in the sense that it allows for the derivation of local entropy or free energy inequalities.

The physical quantities of the system (1) are introduced in Table 1. The mobility coefficients, viscosity coefficients, and the density of the mixture of the fluids depend on the order parameter φ, which reflects the mass concentration of the fluid phases and ranges in the interval $[-1, 1]$.

v	velocity of the fluid	p	fluid pressure
φ	order parameter	μ	chemical potential
$\rho(\varphi)$	fluid density	$\eta(\varphi)$	fluid viscosity
$m(\varphi)$	mobility coefficient	v_a, φ_a	initial states
κ	positive constant	$\varepsilon(v)$	symmetric gradient of v

Table 1: The involved quantities of system (1a)–(1g).

In addition, the Cahn–Hilliard system contains the homogeneous free energy density $\Psi(\varphi) := \Psi_0(\varphi) - \frac{\kappa}{2}\varphi^2$ associated with the underlying Ginzburg-Landau energy, consisting of the convex part $\Psi_0(\varphi)$ and a non-convex contribution $-\frac{\kappa}{2}\varphi^2$ with $\kappa > 0$. In general, the non-convex term enforces the phase separation process, while the convex part serves the purpose of restricting the order parameter φ to the physically meaningful range $[-1,1]$. Depending on the underlying application there are several ways of confining the order parameter to $[-1,1]$ related to different choices of Ψ_0. In this thesis, the focus is mainly on the double-obstacle potential given by

$$\Psi(\varphi) = i_{[-1,1]}(\varphi) - \frac{\kappa}{2}\varphi^2, \tag{2}$$

where $i_{[-1,1]}$ denotes the indicator function of the interval $[-1,1]$. Due to the non-differentiability of $i_{[-1,1]}$, the subdifferential $\partial\Psi_0$ is a multi-valued mapping, which gives rise to a variational inequality in (1b).

The Cahn–Hilliard–Navier–Stokes (CHNS) system (1) arises in a variety of applications, ranging from the solidification process of liquid metal alloys, cf. [62], the simulation of bubble dynamics, as in Taylor flows [9], or pinch-offs of liquid-liquid jets [131], to the formation of polymeric membranes [190] or protein crystallization, see e.g. [132] and references within. Furthermore, the model can be easily adapted to include the effects of colloid particles at fluid-fluid interfaces in gels and emulsions used in food, pharmaceutical, cosmetic or petroleum industries [10, 162]. In many situations it is desirable to control these systems to prescribe a specific behavior, e.g. through a control force u, which acts acts on the right-hand side of the Navier–Stokes equation (1c) or on the boundary condition (1e). This creates the mathematical problem of finding the optimal control $\hat{u}$ out of a given set of admissible controls which realizes the desired behavior in an optimal way.

Due to the presence of a non-smooth homogeneous free energy density, the constraint system of the resulting optimal control problem is generally degenerate. More precisely, classical constraint qualifications (see, e.g., [191]) fail in the optimal control context, preventing the application of the Karush-Kuhn-Tucker theory in Banach spaces for the first-order characterization of an optimal solution by (Lagrange) multipliers. In fact, it is known [111, 118] that the optimal control problem falls into the realm of mathematical programs with equilibrium constraints (MPECs) in function spaces. This problem class is well-known for its constraint degeneracy even in finite dimensions, cf. [142, 160]. As a result, stationarity conditions are no longer unique, compare e.g. [169]. In this context, the main paradigm of this work is that the understanding and proper treatment of the underlying non-smooth problem structure is crucial for both the analytical derivation of stationarity conditions for the optimal control problem as well as the properties of corresponding solution algorithms.

This thesis starts with a preliminary discussion of basic tools from functional analysis, optimization and numerical mathematics in Chapter 1. The covered topics foreshadow the different mathematical fields that are combined later.

Chapter 2 introduces the Cahn–Hilliard–Navier–Stokes model for two-phase flows with non-matched densities. Following the pioneering works [44, 123], there has been an extensive amount of research on the simulation of two-phase flows and their properties. This includes various approaches to extend the model from [123], e.g. for fluids with non-matched densities [3,36,60,141] or surfactants [10,83,162], and the derivation of suitable discretization schemes [8,11,37,81,88–90,93,130] and solvability results [4,5,77,87]. A more detailed overview of the corresponding literature, with more references, is provided in Chapter 2. Moreover, a proper time discretization, which maintains the thermodynamic consistency of the model by allowing for a semi-discrete equivalent of the aforementioned free energy inequalities, is presented. The second part of Chapter 2 establishes the existence of solutions for the original CHNS system as well as for a family of regularized problems at the hands of the Leray-Schauder principle. It is further shown how the intrinsic structure of elliptic variational inequalities and the involved differential operators can be exploited to derive additional regularity properties for the solutions through the use of the corresponding regularity theory for partial differential equations.

The associated optimal control problem is presented in Chapter 3. In contrast to the comparatively rich literature on optimal control of the Cahn–Hilliard system, see e.g. [31,50,51,68,103,117,187,189], the research on optimal control of CHNS systems is very recent and includes only a few publications concerning the two-dimensional case [28,74–76,146], matched densities [118], and smooth free energy densities [82]. In Chapter 3, the existence of globally optimal points is verified via a limit process with respect to an infimizing sequence, followed by a discussion of the analytical and numerical challenges connected to the non-smoothness of the control-to-state operator. In this context, different stationarity concepts for the first-order primal-dual characterization of solutions are investigated. While MPECs and the associated difficulties are already fairly well understood in finite dimensions [142, 160, 169], the literature on infinite dimensional MPECs is comparatively scarce. However, during the last two decades some of the finite-dimensional concepts have been successfully transferred to a function space setting, see e.g. [97, 98, 134]. In general, necessary stationarity conditions for infinite-dimensional problems are either derived by use of penalty and smoothing techniques [18, 19, 27, 73, 125, 137, 181], or with instruments from convex variational analysis and generalized differentiability [26, 113, 148, 149, 151, 152, 159, 186]. The latter usually leads to a form of M- or strong stationarity, while the first approach yields weak or C-stationarity conditions in most cases. A first systematization of stationarity concepts in function spaces was presented in [111], where the concept of ε-almost C-stationarity is introduced.

Expanding on the previous investigations, a Yosida regularization technique with a subsequent passage to the limit with the Yosida parameter is utilized in Chapter 4 to derive conditions of C-stationarity type. This technique is reminiscent of the one pioneered by Barbu in [18], but for different problem classes. In this process, the optimal control of a semi-discrete Cahn–Hilliard–Navier–Stokes system with respect to free energy densities of double-well type is studied and necessary first-order optimality conditions for these problems are derived.

These results are supplemented by the presentation and implementation of a corresponding numerical solution algorithm for the optimal control problem. The various numerical solution methods for this problem class are typically linked to the chosen analytical approach and either rely on the relaxation [111], regularization or penalization [109, 112, 170] of the degeneracy of the lower-level problem and a suitable adjustment of the corresponding (relaxation) parameter, or on a direct characterization/calculation of a generalized derivative of the control-to-state operator [115]. A further collection of algorithms for finite dimensional MPECs including penalty-based interior point methods, piecewise sequential quadratic programming algorithms and descent methods, which relate to an implicit programming approach, is found in the monograph [142] and the references therein. The solver presented in Chapter 4 is based on Moreau-Yosida type approximations of the double-obstacle potential. It includes a mesh adaptation procedure based on a goal-oriented dual-weighted error estimator. Adaptive mesh refinement strategies are an important tool in the simulation and control of both phase field models, where they acknowledge the highly non-uniform structure of solutions [20, 29, 53, 65, 67, 80, 103, 131], as well as Navier–Stokes type equations, where they reduce the numerical expense related to solving the large-scale nonlinear systems upon discretization [58, 84, 122, 135, 136, 180].

Finally, Chapter 5 is devoted to the associated instantaneous control problem, cf. e.g. [79, 119]. Although the control-to-state map of the control problem is generally not differentiable in the sense of, e.g., Gâteau or Fréchet, a so-called conical derivative is available; see e.g. [148, 173]. Expanding on an approach of [127] for the differentiable sensitivity of an elastic contact problem including a viscous membrane, a proper characterization of the conical derivative is obtained. As a result, a more restrictive stationarity system, i.e. strong stationarity, can be targeted based on a methodology similar to [149]. In conjunction with the primal notion of B(ouligand)-differentiability the conical derivative is utilized to create a bundle-free implicit programming method for detecting an approximate solution. Both numerical solvers presented in this thesis are accompanied by a detailed explanation of the numerical realization and the obtained numerical results.

The results from Chapter 2-4 were partly obtained within joint projects with my supervisor M. Hintermüller and D. Wegner [110], and with M. Hintermüller, M. Hinze and C. Kahle [102]. Chapter 5 is based on a preprint with M. Hintermüller which is not yet submitted.

Chapter 1

Mathematical preliminaries: function spaces, optimization, MPECs, variational inequalities and numerical techniques

An introduction to mathematical preliminaries and some general notation for this thesis is presented in this chapter. It is split into several parts. The frequently used function spaces are covered in Section 1.2, whereas Section 1.3 summarizes some useful results from classical optimization theory. Section 1.4 introduces variational inequalities and the related theory, followed by a discussion of a powerful numerical solution method for variational inequalities - the semismooth Newton method - in Section 1.5. In Section 1.6, we take a closer look at optimal control problems where the feasible set is described by a variational inequality and explain the emerging challenges. Finally, we present some basic concepts from numerical analysis and in particular adaptive finite element methods in Section 1.7.

1.1 Notation

For an arbitrary Banach space X equipped with the norm $\|\cdot\|_X$ we denote the closure of a subset $M \subset X$ by $\overline{M}$, its interior by $\mathring{M}$, or $int(M)$, respectively, its boundary by $\partial M = \overline{M} \setminus \mathring{M}$ and its complement by $M^c = X \setminus M$.

The associated *indicator function* $i_M : X \to \mathbb{R} \cup \{\infty\}$ and *characteristic function* $\chi_M : X \to \mathbb{R}$ of M with respect to X are defined by

$$i_M(x) := \begin{cases} 0 \text{ if } x \in M \\ \infty \text{ if } x \notin M \end{cases} \quad \text{and} \quad \chi_M(x) := \begin{cases} 1 \text{ if } x \in M \\ 0 \text{ if } x \notin M \end{cases}, \tag{1.1}$$

respectively. Moreover, the open ball with radius $r > 0$ around a center point $c \in X$ is denoted by $B_r(c) := \{x \in X \mid \|x - c\|_X < r\}$.

We denote the *topological dual space* of X by X^* and $\langle x, x^* \rangle_{X,X^*}$ represents the corresponding duality pairing of $x \in X$ and $x^* \in X^*$. The set $M^\perp$ is defined by

$$M^\perp := \{x^* \in X^* |\ \langle x, x^* \rangle_{X,X^*} = 0,\ \forall\, x \in M\}. \tag{1.2}$$

The strong convergence of a subsequence $\{x_k\}_{k\in\mathbb{N}} \subset X$ to an element $x \in X$ is represented by $x_k \to x$, whereas weak convergence, i.e. convergence with respect to the weak topology, is represented by $x_k \rightharpoonup x$.

We further introduce the Banach space $\mathscr{L}(X,Y)$ of bounded linear operators from X to a Banach space Y. The *adjoint* operator of $A \in \mathscr{L}(X,Y)$ is denoted by $A^* \in \mathscr{L}(Y^*, X^*)$. In addition, $\circ$ denotes the composition operator.

Throughout this thesis, we write $X \hookrightarrow Y$ to signify that an injective mapping $e \in \mathscr{L}(X,Y)$ exists, which embeds X into Y. Additionally, X is called compactly embedded in Y if e is a compact operator, i.e. e maps bounded sets to pre-compact sets.

If Y is a Hilbert space with the inner product $(\cdot,\cdot)_Y$ and $x^* \in Y^*$ is fixed arbitrarily, then there exists a unique $\hat{x} \in Y$ such that $(x, \hat{x})_Y = \langle x, x^* \rangle_{Y,Y^*}$ due to the Riesz representation theorem, which allows us to identify Y and Y^* isometrically. If Y contains a subspace $X \subset Y$ we speak of a *Gelfand triple*

$$X \hookrightarrow Y \cong Y^* \hookrightarrow X^*. \tag{1.3}$$

This will typically be the case for the Sobolev spaces $X = H_0^1(\Omega)$ and $Y = L^2(\Omega)$ introduced in Section 1.2.

Throughout the rest of this text C, C_1, C_2 are generic constants depending only on fixed data and may take different values each time they are used.

1.2 Sobolev spaces and other function spaces

In this section, we introduce several function spaces which will be used throughout the rest of the thesis. For further information on this subject we refer the reader to [7, 42, 144, 145].

We consider a nonempty, open and connected subset $\Omega \subset \mathbb{R}^n$ which we - in accordance with general conventions - also refer to as the *domain*. Furthermore, we assume that Ω is bounded and that the associated boundary $\partial\Omega$ is sufficiently regular. More precisely, we suppose that Ω has the $C^{1,1}$-regularity property given in Definition 1.2.1 below.

For an arbitrary $k \in \mathbb{N} \cup \{0\} \cup \{\infty\}$, we define the space of k-times continuously Fréchet differentiable functions from Ω into $\mathbb{R}^N$ as

$$\begin{aligned}&C^k(\Omega, \mathbb{R}^N)\\ &= \{f : \Omega \to \mathbb{R}^N | f \text{ is } k\text{-times continuously Fréchet differentiable on } \Omega\}.\end{aligned}$$

In particular, $C(\Omega,\mathbb{R}^N) := C^0(\Omega,\mathbb{R}^N)$ and $C^\infty(\Omega,\mathbb{R}^N)$ denote the space of continuous functions on Ω and the space of infinitely Fréchet differentiable functions on Ω. The space $C_0^k(\Omega,\mathbb{R}^N)$ represents the subspace of $C^k(\Omega,\mathbb{R}^N)$ which consists of all functions $f \in C^k(\Omega,\mathbb{R}^N)$ with compact support in Ω. Moreover, we introduce the space of k-times continuously Fréchet differentiable functions up to the boundary of Ω as

$$\begin{aligned}&C^k(\overline{\Omega}, \mathbb{R}^N)\\ &= \{f \in C^k(\Omega, \mathbb{R}^N) | \partial_\iota f \text{ has a continuous extension to } \overline{\Omega}, \forall \iota \in \mathbb{N}^n |\iota|_1 \leq k\},\end{aligned}$$

where $\iota = (\iota_1, .., \iota_n) \in \mathbb{N}^n$ denotes a suitable multi-index and $|\iota|_p$ denotes the standard p-norm in $\mathbb{R}^n$ with $1 \leq p \leq \infty$. In the following, we usually omit the subscript p when $p = 2$.

For $0 < \alpha \leq 1$, the subspace $C^{k,\alpha}(\overline{\Omega},\mathbb{R}^N)$ of $C^k(\overline{\Omega},\mathbb{R}^N)$ contains all functions of $C^k(\overline{\Omega},\mathbb{R}^N)$ whose partial derivatives of order k are Hölder continuous with the Hölder constant $0 < \alpha < 1$ or Lipschitz continuous (for $\alpha = 1$), respectively. In the case of $N = 1$, we use the notation $C^k(\Omega) := C^k(\Omega,\mathbb{R})$.

This concludes the tools necessary to provide a rigorous definition of the $C^{k,\alpha}$*-regularity property* mentioned above.

Definition 1.2.1 ($C^{k,\alpha}$-regularity property)**.** *Let $k \in \mathbb{N}$ and $\iota \in [0,1]$. Then a bounded domain Ω has the $C^{k,\alpha}$-regularity property if there exists $M \in \mathbb{N}$ such that for every $1 \leq i \leq M$, an orthonormal basis $\{b_{i,1}, .., b_{i,n}\}$ of $\mathbb{R}^n$, a constant $R_i > 0$ and a function $f_i \in C^{k,\alpha}(\overline{B_{r_i}(c_i)})$ on a ball around $c_i \in \mathbb{R}^{n-1}$ with radius $r_i > 0$ can* *be found such that the family of sets $\{\Omega_1,..,\Omega_M\}$, where Ω_i is defined as*

$$\Omega_i = \{x = \sum_{j=1}^{n} x_{i,j} b_{i,j} \;\Big|\; |\hat{x}_i^{-n} - c| < r_i \wedge |x_{i,n} - f_i(\hat{x}_i^{-n})| < R_i\}, \tag{1.4}$$

(with $\hat{x}_i^{-n} := (x_{i,1},..,x_{i,n-1})$) satisfies the following conditions

$$\partial\Omega \subset \bigcup_{i=1}^{M} \Omega_i, \tag{1.5}$$

$$\Omega_i \cap \partial\Omega = \{x \in \mathbb{R}^n \mid |\hat{x}_i^{-n} - c_i| < r_i, x_{i,n} = f_i(\hat{x}_i^{-n})\}, \tag{1.6}$$

$$\Omega_i \cap \Omega = \{x \in \mathbb{R}^n \mid |\hat{x}_i^{-n} - c_i| < r_i, x_{i,n} > f_i(\hat{x}_i^{-n})\}, \tag{1.7}$$

$$\Omega_i \cap \Omega^c = \{x \in \mathbb{R}^n \mid |\hat{x}_i^{-n} - c_i| < r_i, x_{i,n} < f_i(\hat{x}_i^{-n})\}. \tag{1.8}$$

At this point, we also introduce the Fourier transform.

Definition 1.2.2. *The Fourier transform $\mathscr{F}[f]$ of a function $f : \mathbb{R} \to H$ into a Hilbert space H is given by*

$$\mathscr{F}[f](x) := \int_{-\infty}^{\infty} e^{-2i\pi xy} f(y)dy. \tag{1.9}$$

Sobolev spaces

For arbitrary $p \in \mathbb{R}$ with $1 \leq p$, we denote by $L^p\left(\Omega, \mathbb{R}^N\right)$ the space of all (Lebesgue) measurable functions $f : \Omega \to \mathbb{R}^N$ for which the norm

$$\|f\|_{L^p} := \left(\int_\Omega |f(x)|^p \, dx\right)^{\frac{1}{p}} \tag{1.10}$$

is finite. We identify functions that are equal almost everywhere (a.e.) on Ω. As above, we omit the indication of $\mathbb{R}^N$ if $N = 1$.

We say that $f : \Omega \to \mathbb{R}^N$ is locally p-integrable and write $f \in L^p_{loc}(\Omega, \mathbb{R}^N)$ if

$$\int_K |f(x)|^p \, dx < \infty$$

for all compact subsets $K \subset \Omega$.

For $p = \infty$ we denote by $L^\infty\left(\Omega, \mathbb{R}^N\right)$ the space of all functions $f : \Omega \to \mathbb{R}^N$ which are essentially bounded on Ω, i.e. there exists a constant B such that $|f(x)| \leq B$, a.e. on Ω. The L^∞-norm of f is then defined as the infimum of all such constants B

$$\|f\|_{L^\infty} := \operatorname*{ess\,sup}_{x\in\Omega} |f(x)|. \tag{1.11}$$

For $p > 1$ we call $p' := p/(p-1)$ the *conjugate exponent* to p. If $p = 1$, we formally define $p' := \infty$ and vice versa. Due to Hölder's inequality, it holds that

$$\int_\Omega f(x)\, g(x)\, dx \leq \|f\|_{L^p} \|g\|_{L^{p'}} \tag{1.12}$$

for every $f \in L^p\left(\Omega, \mathbb{R}^N\right)$ and $g \in L^{p'}\left(\Omega, \mathbb{R}^N\right)$. We now characterize the dual space of $L^p\left(\Omega, \mathbb{R}^N\right)$.

Lemma 1.2.1 (Dual space of $L^p(\Omega, \mathbb{R}^N)$). *Let $p \geq 1$ and p' be its conjugate exponent. Then for each $L \in \left[L^p\left(\Omega, \mathbb{R}^N\right)\right]^*$ there exists $l \in L^{p'}\left(\Omega, \mathbb{R}^N\right)$ such that for all $f \in L^p\left(\Omega, \mathbb{R}^N\right)$, it holds that*

$$L(f) = \int_\Omega l(x)\, f(x)\, dx. \tag{1.13}$$

Moreover, $L^{p'}\left(\Omega, \mathbb{R}^N\right) \cong \left[L^p\left(\Omega, \mathbb{R}^N\right)\right]^*$.

Note that $L^2\left(\Omega, \mathbb{R}^N\right)$ is a Hilbert space with respect to the inner product

$$\langle f, g\rangle_{L^2} = \int_\Omega f(x)\, g(x)\, dx. \tag{1.14}$$

We therefore identify $L^2(\Omega, \mathbb{R}^N)$ with its dual space as described in Section 1.1. Furthermore, $L^p\left(\Omega, \mathbb{R}^N\right)$ is reflexive if $1 < p < \infty$ and separable if $1 \leq p < \infty$.

For $k \in \mathbb{N}$ and $1 \leq p \leq \infty$ we introduce the norm

$$\|f\|_{k,p} := \left(\sum_{0 \leq |\iota| \leq k} \|\partial_\iota f\|_{L^p}\right)^{1/p}, \tag{1.15}$$

and define the classical *Sobolev space* $W^{k,p}(\Omega)$ as the completion of the set $\left\{f \in C^k(\Omega) \,|\, \|f\|_{W^{k,p}} < \infty\right\}$ with respect to the norm $\|\cdot\|_{k,p}$. For $m \in \mathbb{N}$ and the multi-index $\iota \in \mathbb{N}^m$ v_ι is called a *weak partial derivative* of $f \in L^p(\Omega)$, which is denoted by $\partial_\iota f = v_\iota$, if it satisfies

$$\int_\Omega f(x)\, \partial_\iota h(x)\, dx = (-1)^{|\iota|} \int_\Omega v_\iota(x)\, h(x)\, dx, \quad \forall h \in C_0^\infty(\Omega). \tag{1.16}$$

In this context, we usually refer to h as a *test function*. At this point, we introduce the gradient ∇f and the symmetrized gradient $\varepsilon(f)$ of f as follows

$$\nabla f = (\partial_1 f, .., \partial_N f)^\top, \; \varepsilon(f) := \frac{1}{2}(\nabla f + \nabla f^\top). \tag{1.17}$$

Alternatively, $W^{k,p}(\Omega)$ can be defined as the collection of all functions $f \in L^p(\Omega)$, whose weak derivatives $\partial_\iota f$ of order $|\iota| \leq k$ also belong to $L^p(\Omega)$. By regarding $W^{k,p}(\Omega)$ as a closed subspace of the Cartesian product of $L^p(\Omega)$-spaces, it can easily be verified that many properties are transferred from the associated $L^p(\Omega)$-spaces. Namely, $W^{k,p}(\Omega)$ is reflexive, respectively, separable if $L^p\left(\Omega, \mathbb{R}^N\right)$ is.

During our study of partial differential equations, the boundary values at $\partial\Omega$ will often be of special interest. Since Ω has the $C^{1,1}$-regularity property, there exists a *trace mapping* $\gamma \in \mathscr{L}(W^{k,p}(\Omega), W^{k-1,p}(\partial\Omega))$ such that $\gamma(f)$ is equal to the restriction of f to $\partial\Omega$, i.e. $f_{|\partial\Omega}$, for every $f \in W^{k,p}(\Omega)) \cap C^{k-1}\left(\overline{\Omega}\right))$.

Next, we introduce the subspaces $W_0^{k,p}(\Omega)$ as the closure of $C_0^\infty(\Omega)$ in $W^{k,p}(\Omega)$ and observe that $f \in W_0^{1,p}(\Omega)$ if and only if $f_{|\partial\Omega} \equiv 0$, *a.e.* $\partial\Omega$. Furthermore, the functional

$$\|f\|_{W_0^{k,p}} = \left(\sum_{|\iota|=k} \|\partial_\iota f\|_{L^p}\right)^{1/p} \tag{1.18}$$

defines an equivalent norm in $W_0^{k,p}(\Omega)$. In addition, we introduce the following Sobolev spaces with mean value zero

$$\overline{W}^{k,p}(\Omega) = \left\{ f \in W^{k,p}(\Omega) | \int_\Omega f dx = 0 \right\}; \tag{1.19a}$$

$$\overline{W}^{k,p}_{\partial_n}(\Omega) = \left\{ f \in \overline{W}^{k,p}(\Omega) | \partial_n f_{|\partial\Omega} = 0 \text{ a.e. on } \partial\Omega \right\},\ k \geq 2. \tag{1.19b}$$

The spaces $W^{k,2}(\Omega)$, $W_0^{k,2}(\Omega)$, and $\overline{W}^{k,2}_{\partial_n}(\Omega)$ are Hilbert spaces and will from now on be abbreviated by $H^k(\Omega)$, $H_0^k(\Omega)$, and $\overline{H}^k_{\partial_n}(\Omega)$, respectively.

Accordingly, the Sobolev spaces $W^{k,p}\left(\Omega, \mathbb{R}^N\right)$ and $W_0^{k,p}\left(\Omega, \mathbb{R}^N\right)$ are defined component-wise.

Hereafter, we provide some useful embedding properties of Sobolev spaces for future application, cf. e.g. [7].

Theorem 1.2.1 (Sobolev Imbedding Theorem). *For $j, k \in \mathbb{N}$ and $1 \leq p < \infty$ with $kp > n$, it holds that*

$$W^{j+k,p}(\Omega) \hookrightarrow C^j\left(\overline{\Omega}\right) \tag{1.20}$$

and

$$W^{j+k,p}(\Omega) \hookrightarrow W^{j,q}(\Omega) \tag{1.21}$$

for $1 \leq q \leq \infty$.
If $kp = n$, then the embedding (1.21) is valid for $1 \leq q < \infty$.
If $kp < n$, then the embedding (1.21) is valid for $p \leq q \leq \frac{np}{n-kp}$.

Remark 1.2.1. *Theorem 1.2.1 still holds true if we replace the space $C^j\left(\overline{\Omega}\right)$ in (1.20) by $C^{j,\alpha}\left(\overline{\Omega}\right)$ for suitable $0<\alpha<1$. For $q=\infty$, it holds that $u\in W^{1,\infty}(\Omega)$ if and only if there exists a Lipschitz continuous function v on $\overline{\Omega}$ which coincides with u a.e. on Ω.*

In fact, most of the embedding operators described in Theorem 1.2.1 are compact.

Theorem 1.2.2 (Rellich Kondrachov Theorem). *The embeddings given in Theorem 1.2.1 are compact for $q<\infty$. The assertion still holds true if we replace $W^{j+k,p}(\Omega)$ by $W_0^{j+k,p}(\Omega)$.*

As a consequence, the spaces $H_0^1(\Omega)$, $L^2(\Omega)$ and $H^{-1}(\Omega):=(H_0^1(\Omega))^*$ form a *Gelfand triple*

$$H_0^1(\Omega)\hookrightarrow L^2(\Omega)\hookrightarrow H^{-1}(\Omega), \tag{1.22}$$

where both embeddings are compact.

In our analytical treatment of the Cahn-Hilliard-Navier-Stokes system and the incompressible Navier-Stokes equation in particular, we will frequently encounter solenoidal vector fields. For this reason, we introduce the Hilbert space

$$H_\sigma(\Omega):=\left\{f\in L^2(\Omega,\mathbb{R}^N)|\mathrm{div}f=0,\ \text{a.e. on }\Omega\right\} \tag{1.23}$$

and the associated inner product

$$(f,g)_{H_\sigma}=(f,g)_{L^2(\Omega,\mathbb{R}^N)}+(\mathrm{div}(f),\mathrm{div}(g))_{L^2}. \tag{1.24}$$

Here, div denotes the standard divergence operator

$$\mathrm{div}(f):=\sum_{i=1}^N\partial_i(f_i). \tag{1.25}$$

Making use of the $C^{1,1}$-regularity property of Ω once more, we note the existence of a trace mapping $\hat{\gamma}:H_\sigma(\Omega)\to H^{-\frac{1}{2}}(\partial\Omega)$, where $H^{-\frac{1}{2}}(\partial\Omega)$ represents the dual space of the Hilbert space $H^{\frac{1}{2}}(\partial\Omega)$ of trace functions of $H_0^1(\Omega)$, i.e. $H^{\frac{1}{2}}(\partial\Omega):=\gamma(H_0^1(\Omega))\subset L^2(\partial\Omega)$.

We further observe that the image space of the gradient operator, i.e. $G(\Omega):=\nabla(H_0^1(\Omega))$, is a closed Hilbert space equipped with the inner product $(\cdot,\cdot)_{L^2(\Omega,\mathbb{R}^N)}$. There exists an orthogonal decomposition of $L^2(\Omega,\mathbb{R}^N)$ into $G(\Omega)$ and the space of divergence free vector fields, i.e.

$$(L^2(\Omega))^n=G(\Omega)\oplus H_\sigma(\Omega). \tag{1.26}$$

With the help of (1.23) we introduce the space $H^k_{0,\sigma}(\Omega;\mathbb{R}^N)$ for arbitrary $k \in \mathbb{N}$ via

$$H^k_{0,\sigma}(\Omega;\mathbb{R}^N) = H^k_0(\Omega;\mathbb{R}^N) \cap H_\sigma(\Omega). \tag{1.27}$$

Since the Cahn-Hilliard-Navier-Stokes system describes the evolution of two-phase flows over time, we must also consider time-dependent functions and the associated Sobolev spaces introduced below. For a Banach space X and a time interval $(0,T)$ we define the time-dependent Sobolev space $L^p(0,T;X)$ as the space of all functions $f : (0,T) \to X$ such that the norm

$$\|f\|_{L^p(0,T;X)} := \left(\int_0^T \|f(t)\|_X^p \, dt \right)^{\frac{1}{p}} \tag{1.28}$$

is finite. In the subsequent investigations X will usually be a spatial Sobolev space itself, e.g., $X = L^2(\Omega)$ or $X = H^1_0(\Omega)$.

A function $f \in L^1(0,T;X)$ is called weakly differentiable (with respect to time), if and only if there exists a weak derivative g - denoted by $\dot{f} = g$ - satisfying

$$\int_0^T f(t)h'(t)dt = -\int_0^T g(t)h(t)dt \tag{1.29}$$

for every $h \in C_0^\infty(0,T)$. Then $W^{1,p}(0,T;X)$ is defined as the space of all functions $f \in L^p(0,T;X)$, which possess a weak derivative $\dot{f} \in L^p(0,T;X)$, and is equipped with the norm

$$\|f\|_{W^{1,p}(0,T;X)} := \left(\|f\|^p_{L^p(0,T;X)} + \|\dot{f}\|^p_{L^p(0,T;X)} \right)^{\frac{1}{p}}. \tag{1.30}$$

We note that most of the properties of spatial Sobolev spaces presented above can be directly transfered to their time-dependent equivalents.

Next, we briefly introduce the function spaces BMO and VMO of functions with bounded mean oscillation and vanishing mean oscillation, respectively.

Definition 1.2.3 (BMO space). *For a locally integrable function $f : \mathbb{R}^n \to \mathbb{R}$ the mean oscillation of f over a ball $B_r(y) \subset \mathbb{R}^n$ with $y \in \mathbb{R}^n$ and $r > 0$ is given by*

$$\frac{1}{|B_r(y)|} \int_{B_r(y)} \left| f(x) - f_{B_r(y)} \right| dx, \tag{1.31}$$

where $|B_r(y)|$ denotes the Lebesgue measure of $B_r(y)$, and

$$f_{B_r(y)} := \frac{1}{|B_r(y)|} \int_{B_r(y)} f(x)dx. \tag{1.32}$$

We say that f has a bounded mean oscillation, i.e. $f \in BMO$, if

$$\|f\|_{BMO} := \sup_{y \in \mathbb{R}^n, r>0} \frac{1}{|B_r(y)|} \int_{B_r(y)} \left| f(x) - f_{B_r(y)} \right| dx < \infty. \tag{1.33}$$

BMO is a Banach space if equipped with the norm $\|\cdot\|_{BMO}$.

Definition 1.2.4 (VMO space). *For $f \in BMO$ and $r > 0$ we set*

$$\eta_f(r) := \sup_{y \in \mathbb{R}^n, \rho \leq r} \frac{1}{|B(y,\rho)|} \int_{B(y,\rho)} \left| f(x) - f_{B(y,\rho)} \right| dx. \tag{1.34}$$

A function $f \in BMO$ lies in VMO if

$$\lim_{r \to 0} \eta_f(r) = 0. \tag{1.35}$$

We refer to $\eta_f(r)$ as the VMO-modulus of f.

As pointed out in [144], the space of vanishing mean oscillation plays a similar role in BMO, as the space of bounded uniformly continuous functions in $L^\infty(\Omega)$. Indeed, condition (1.35) represents a kind of continuity in the average sense and not in the pointwise sense.

Theorem 1.2.3. *Let $f \in BMO$, $z \in \mathbb{R}$ and $f_z : \mathbb{R}^n \to \mathbb{R}$ be given by $f_z(x) := f(x-z)$. Then the following conditions are equivalent:*

(1) $f \in VMO$,

(2) *For any $\varepsilon > 0$ there exists a uniformly continuous function $g : \mathbb{R}^n \to \mathbb{R}$ such that $\|f - g\|_{BMO} < \varepsilon$,*

(3) $\lim_{z \to 0} \|f_z - f\|_{BMO} = 0$.

We point out that every uniformly continuous function has vanishing mean oscillation, since the VMO-modulus can be estimated from above by the modulus of continuity.

1.3 Optimization

The classical problem in optimization theory is to find a point $\bar{x}$ which solves the minimization problem

$$\min_{x \in M} f(x). \tag{1.36}$$

Here, $M \subset X$ is called the *feasible set* and f is a real-valued function on M called the *objective functional*. A point $\bar{x} \in M$ is called *optimal* if it is a solution to the problem (1.36).

In order to ensure the existence of such an optimal point, it is usually necessary to impose additional assumptions on the objective f or the feasible set M.

Definition 1.3.1 (Coercivity)**.** *A function $f : X \to Y$ from a normed space X into a normed space Y is called coercive, if*

$$\|f(x)\|_Y \to \infty \text{ for } \|x\|_X \to \infty. \tag{1.37}$$

The subsequent theorem guarantees the existence of solutions to (1.36) in a rather general setting, see e.g. [35]. It includes the case of infinity-valued functions, i.e. $f(x) \in \overline{\mathbb{R}} := \mathbb{R} \cup \{-\infty, \infty\}$.

Theorem 1.3.1 (Weierstraß theorem)**.** *Let X be a reflexive Banach space and M a weakly closed subset of X. Further assume that $f : M \to \overline{\mathbb{R}}$ is weakly lower-semicontinuous and bounded from below. If either M is bounded or f is coercive, then the problem* (1.36) *possesses at least one solution.*

Remark 1.3.1. *Theorem 1.3.1 applies to a variety of situations. In particular, we note that*

1. *if M is closed and convex, then it is weakly closed;*

2. *if f is convex and continuous, then it is weakly lower-semicontinuous.*

In the subsequent chapters, we employ a similar argumentation as in Theorem 1.3.1 to ensure the existence of solutions to the optimization problems under investigation.

Variational concepts in convex analysis

In this subsection, we briefly introduce some analytic concepts which will be used in the next sections and throughout the rest of this work. More information can be found e.g. in [63, 151, 152]. We assume that the subset $M \subset X$ is non-empty, closed and convex. The subsequent definition introduces various different cones associated to the set M,.

Definition 1.3.2 (Conical hull, polar cone, normal cone, tangent cone, radial cone, critical cone)**.** *The conical hull of the set M is defined by*

$$con(M) := \{\alpha \cdot x |\, x \in M,\ \alpha \geq 0\}. \tag{1.38}$$

The polar cone of the set M is defined by

$$M^0 := \{x^* \in X^* |\, \langle x^*, y\rangle \leq 0,\ \forall y \in M\}. \tag{1.39}$$

The normal cone of M at a point $\hat{x} \in M$ is given by

$$N_M(\hat{x}) := \{x^* \in X^* |\, \langle x^*, y - \hat{x}\rangle \leq 0,\ \forall y \in M\} \subset X^*. \tag{1.40}$$

The tangent cone of M at $\hat{x} \in M$ is given by

$$T_M(\hat{x}) := \{v \in X | \exists\, t_k > 0, t_k \to 0, \exists\, v_k \in X, v_k \to v, \forall\, k \in \mathbb{N} : \hat{x} + t_k v_k \in M\}. \tag{1.41}$$

Note that the tangent is sometimes also referred to as the contingent cone.

The radial cone of M at $\hat{x} \in M$ is given by

$$R_M(\hat{x}) := \{v \in X |\ \exists\, \bar{t} > 0, \forall\, 0 \leq t \leq \bar{t} : \hat{x} + tv \in M\}. \tag{1.42}$$

For a given $x^* \in N_M(\hat{x})$, the critical cone associated to M, $\hat{x}$ and x^* is defined by

$$\mathscr{K}(\hat{x}, x^*) := T_M(\hat{x}) \cap \{x^*\}^\perp. \tag{1.43}$$

The above cones are closely intertwined and play an important role in convex optimization theory. In particular, we mention the following relations

$$N_M(\hat{x}) = [T_M(\hat{x})]^0, \tag{1.44}$$
$$\overline{R_M(\hat{x})} = T_M(\hat{x}), \tag{1.45}$$
$$\mathscr{K}(\hat{x}, x^*) \subset T_M(\hat{x}),\ \forall\, x^* \in N_M(\hat{x}), \tag{1.46}$$
$$v \in N_{\mathscr{K}(\hat{x},x^*)}(h) \Leftrightarrow h \in \mathscr{K}(\hat{x}, x^*) \wedge v \in [\mathscr{K}(\hat{x}, x^*)]^0 \wedge \langle v, h\rangle = 0. \tag{1.47}$$

Definition 1.3.3 (polyhedric)**.** *The closed, convex set M is called polyhedric, if for every $\hat{x} \in M$ and $x^* \in N_M(\hat{x})$ it holds that*

$$\mathscr{K}(\hat{x}, x^*) = \overline{R_M(\hat{x}) \cap \{x^*\}^\perp}. \tag{1.48}$$

At this point, we also introduce the following generalized differentiability concept for arbitrary convex functions, along with the associated calculus rules.

Definition 1.3.4 (Subdifferential)**.** *Let $f : X \to \mathbb{R} \cup \{\infty\}$ be a convex, lower semi-continuous function. Then the subdifferential ∂f of f at a point $x \in X$ is defined by*

$$\partial f(x) := \{x^* \in X^* : f(y) \geq f(x) + \langle x^*, y - x\rangle \, \forall y \in X\}. \tag{1.49}$$

Furthermore, $x^* \in \partial f(x)$ is called a subgradient of f at x.

Lemma 1.3.1 (Subdifferential calculus)**.** *Let $f_1, f_2 : X \to \mathbb{R} \cup \{\infty\}$ be convex, lower semi-continuous functions, $l : Y \to X$ be a continuous linear mapping and $\hat{x}_1 \in$ $\mathrm{dom} f_1 \cap \mathrm{dom} f_2$ such that f_1 is continuous at $\hat{x}_1$. Further assume that there exists a point $\hat{x}_2$ such that f_1 is continuous and finite at $l(\hat{x}_2)$.*

Then it holds for every $x \in X$ that:

$$\partial(cf_1)(x) = c\partial f(x), \quad \forall c > 0, \tag{1.50}$$

$$\partial(f_1 + f_2)(x) = \partial f_1(x) + \partial f_2(x), \tag{1.51}$$

$$\partial(f_1 \circ l)(x) = l^* \partial f_1(l(x)). \tag{1.52}$$

It is easy to see that the normal cone of M at $\hat{x}$ can be rewritten as the subdifferential of the associated indicator function, i.e.

$$N_M(\hat{x}) = \partial i_M(\hat{x}). \tag{1.53}$$

The relation between the concepts of Gateaux differentiability and subdifferentiability is clarified in the following theorem.

Theorem 1.3.2. *Let $f : X \to \mathbb{R} \cup \{\infty\}$ be a convex function. If f is Gateaux differentiable at a point $x \in X$, then it is subdifferentiable at x and $\partial f(x) = \{Df(x)\}$, where $Df(x)$ denotes the associated Gateaux derivative. Conversely, if f is continuous and finite and has a single-valued subgradient at the point $x \in X$, then f is Gateaux differentiable at x with $Df(x) \in \partial f(x)$.*

We briefly present a powerful tool when it comes to the stability analysis of optimization problems.

Definition 1.3.5. *A family of functionals $f_\alpha : X \to [-\infty, \infty]$ is said to Γ-converge to $f : X \to [-\infty, \infty]$ for $\alpha \to 0$ if and only if the following statements are satisfied.*

1. *For every convergent sequence $\{x_\alpha\}_{\alpha > 0} \subset X$ and the associated limit point $\bar{x}$, it holds that*

$$f(\bar{x}) \leq \liminf_{\alpha \to 0} f_\alpha(x_\alpha). \tag{1.54}$$

2. *For every $\bar{x} \in X$ there exists a sequence $\{x_\alpha\}_{\alpha>0} \subset X$ which converges to $\bar{x}$ such that*

$$f(\bar{x}) \geq \limsup_{\alpha \to 0} f_\alpha(x_\alpha). \tag{1.55}$$

For more details on the subject we refer the reader to [14] and the pioneering works of De Giorgi [54, 55].

First-order optimality conditions

In this section, we discuss different ways to better characterize the solutions to (1.36). In particular, we present necessary optimality conditions which have to be satisfied in order for a point $x \in X$ to be optimal. Further details on the subject can be found e.g. in [34, 35, 63, 167, 191]

By the definition of the subdifferential it is clear that a solution $\bar{x}$ to the unconstrained problem (1.36), i.e. if $M = X$, is equivalently described by the inclusion

$$0 \in \partial f(\bar{x}), \tag{1.56}$$

if f is convex and lower semi-continuous.

Suppose that f can be expressed as follows

$$f(x) := f_1(l(x)) + f_2(x), \tag{1.57}$$

where f_1, f_2 and l satisfy the assumptions made in Lemma 1.3.1. In particular, we assume that the following constraint qualification is satisfied

$$0 \in \mathit{int}(\mathrm{dom} f_1 - l(\mathrm{dom} f_2)). \tag{1.58}$$

Then, inclusion (1.56) transforms into

$$0 \in l^* \partial f_1(l(\bar{x})) + \partial f_2(\bar{x}), \tag{1.59}$$

where we used the calculus rules from Lemma 1.3.1.

This result can be applied to the initial problem (1.36) by formulating it as the following unconstrained optimization problem

$$\min_{x \in X} f(x) + i_M(x). \tag{1.60}$$

If f is Gateaux differentiable, we obtain a characterization of an optimal point $\bar{x}$

$$-Df(\bar{x}) \in \partial i_M(\bar{x}) = N_M(\bar{x}). \tag{1.61}$$

This is depicted in the following theorem.

Theorem 1.3.3. *Let X be a reflexive Banach space and $M \subset X$ a non-empty closed convex set. Suppose that f is Gateaux differentiable functional on X.*

If $\bar{x}$ solves (1.36)*, then*

$$\langle Df(\bar{x}), y - \bar{x} \rangle \geq 0, \quad \forall y \in M. \tag{1.62}$$

If f is also convex, then both statements are equivalent.

Condition (1.62) is called a variational inequality. We take a closer look on these inequalities in the next section.

If additional knowledge about the structure of the feasible set M is available, the necessary optimality conditions can be further specified. This is briefly illustrated at the hands of the following finite dimensional optimization problem

$$\min_{x \in \mathbb{R}^n} f(x), \ s.t. \ x \in M = \{x \in \mathbb{R}^n | \ g_i(x) \leq 0 \ \forall i = 1,..,m\} \tag{1.63}$$

where f, g_i are real-valued, continuously differentiable functions on $\mathbb{R}^n$.

Definition 1.3.6 (Lagrange function, saddle point)**.** *The Lagrange function or Lagrangian $L : \mathbb{R}^n \times \mathbb{R}^m \to \mathbb{R}$ associated to* (1.63) *is defined by*

$$L(x, \lambda) := f(x) + \sum_{i=1}^{m} \lambda_i g_i(x). \tag{1.64}$$

The pair $(\bar{x}, \overline{\lambda}) \in \mathbb{R}^n \times \mathbb{R}^m$ with $\overline{\lambda}_i \geq 0$, $\forall 1 \leq i \leq m$ is called a saddle point of L, if

$$L(x, \overline{\lambda}) \geq L(\bar{x}, \overline{\lambda}) \geq L(\bar{x}, \lambda), \quad \forall (x, \lambda) \in \mathbb{R}^n \times \mathbb{R}^m, \ \lambda \geq 0. \tag{1.65}$$

If $(\bar{x}, \overline{\lambda})$ is a saddle point of L, then $\bar{x}$ solves the problem (1.63).

In general, it is, however, unclear whether a locally optimal point of (1.63) necessarily satisfies a Karush-Kuhn-Tucker type system. This can only be guaranteed if the given data fulfills a constraint qualification as, e.g., the Mangasarian-Fromovitz constraint qualification (MFCQ) or the strict MFCQ defined below.

Definition 1.3.7 (MFCQ and SMFCQ)**.** *We say that the the MFCQ holds at a point $\hat{x} \in \mathbb{R}^n$ if there exists a vector v such that*

$$\nabla g_i(\hat{x}) v < 0, \quad \forall i : g_i(\hat{x}) = 0. \tag{1.66}$$

We further say that the SMFCQ is satisfied if there exist Lagrange multipliers Λ, λ, μ such that the set $\{\nabla g_i(\hat{x}), \ i : \lambda_i > 0\}$ is linearly independent and there exists a vector v such that

$$\nabla g_i(\hat{x}) v = 0, \quad \forall i : \lambda_i > 0, \tag{1.67}$$

$$\nabla g_i(\hat{x}) v < 0, \quad \forall i : g_i(\hat{x}) = \lambda_i = 0. \tag{1.68}$$

Then the subsequent theorem provides necessary (first-order) optimality conditions for a solution of (1.63).

Theorem 1.3.4 (Karush-Kuhn-Tucker conditions)**.** *Let $\overline{x}$ be a locally optimal point of* (1.63) *and suppose that a constraint qualification holds true.*

Then there exists a Lagrange multiplier $\overline{\lambda} \in \mathbb{R}^m$ such that the following Karush-Kuhn-Tucker conditions are satisfied

$$\overline{\lambda}_i \geq 0, \quad \forall i = 1,..,m, \tag{1.69a}$$

$$\overline{\lambda}_i g_i(\overline{x}) = 0, \quad \forall i = 1,..,m, \tag{1.69b}$$

$$D_x L(\overline{x}, \overline{\lambda}) = Df(\overline{x}) + \sum_{i=1}^{m} \overline{\lambda}_i Dg_i(\overline{x}) = 0. \tag{1.69c}$$

The proof is based on the application of the Hahn-Banach separation theorem to the linearized problem

$$\min_{x \in \mathbb{R}^n} f(\overline{x}) + Df(\overline{x})(x - \overline{x}), \tag{1.70}$$

$$s.t. \; g_i(\overline{x}) + Dg_i(\overline{x})(x - \overline{x}) \leq 0, \quad i = 1,..,m, \tag{1.71}$$

which guarantees the existence of a vector $\begin{pmatrix} \lambda_0 \\ \lambda \end{pmatrix} \in \mathbb{R}^{m+1}$ such that

$$\lambda_0 Df(\overline{x})(x - \overline{x}) + \sum_{i=1}^{m} \lambda_i Dg_i(\overline{x})(x - \overline{x}) = 0, \quad \forall x \in \mathbb{R}^n. \tag{1.72}$$

Then the constraint qualification ensures that $\lambda_0 \neq 0$.

In our subsequent studies we transfer the concepts of Lagrangians and Lagrange multipliers to infinite-dimensional problems. For this purpose, we partly rely on the results of [191], where the existence of Lagrange multipliers was established in a more general Banach space setting. The authors studied the problem

$$\min f(x), \text{ s.t. } x \in M, \; g(x) \in K, \tag{1.73}$$

where X and Y are real Banach spaces, f is a Fréchet differentiable functional on X, and the function $g : X \to Y$ is continuously Fréchet differentiable. As above, $M \subset X$ is a non-empty, closed and convex subset and K is a closed, convex cone in Y with vertex at the origin. Let $M(x)$ and $K(y)$ denote the *conical hull* of the sets $M - \{x\}$ and $K - \{y\}$, respectively, i.e.

$$M(x) := con(M - \{x\}) = \{\alpha(c - x) \mid c \in M, \; \alpha \geq 0\}, \tag{1.74}$$

$$K(y) := con(K - \{y\}) = \{k - \alpha y \mid k \in K, \; \alpha \geq 0\}. \tag{1.75}$$

Definition 1.3.8 (Lagrange multiplier)**.** *Let $\overline{x} \in X$ be a locally optimal point of the problem* (1.73)*. We say that $\lambda \in Y^*$ is a Lagrange multiplier at $\overline{x}$, if*

$$\lambda \in K^+, \tag{1.76a}$$

$$\langle \lambda, g(\overline{x}) \rangle = 0, \tag{1.76b}$$

$$Df(\overline{x}) - \lambda \circ Dg(\overline{x}) \in M(\overline{x})^+. \tag{1.76c}$$

In [191, Theorem 4.1], it has been shown that the existence of Lagrange multipliers can be guaranteed for an optimal point $\overline{x} \in X$ of (1.73), if the problem satisfies the regularity assumption (1.77).

Theorem 1.3.5. *Let $\overline{x} \in X$ be an optimal solution for* (1.73) *and assume that the following constraint qualification is satisfied*

$$Dg(\overline{x})M(\overline{x}) - K(g(\overline{x})) = Y. \tag{1.77}$$

Then the set of Lagrange multipliers at $\overline{x}$ is non-empty and bounded.

Note that the system (1.76) constitutes the infinite dimensional counterpart of the system (1.69) and the constraint qualification (1.77) translates to the MFCQ (1.66) in finite dimensions.

The proof uses a generalization of the open mapping theorem (cf. [191, Theorem 2.1]) to ensure that the linearizing cone of M at $\overline{x}$

$$L_M(\overline{x}) := \{v \in X \mid v \in M(\overline{x}) \wedge Dg(\overline{x})v \in K(g(\overline{x}))\} \tag{1.78}$$

is contained in the sequential tangent cone $T_M(\overline{x})$ at $\overline{x}$ if (1.77) is satisfied.

1.4 Variational inequalities

As seen in the previous section, the study of optimization problems often leads to the formulation of variational inequalities, see, e.g. (1.62). In the course of this thesis, we thoroughly analyse the properties of a specific variational inequality, the so-called Cahn-Hilliard equation. Subsequently, we present a general introduction to these inequalities and discuss the existence and uniqueness of corresponding solutions. For more information we refer to e.g. [18, 133, 139].

Maintaining the above notation, we consider a Hilbert space H, a non-empty subset $M \subset H$ and an operator $F : M \to H^*$. The inequality

$$\langle F(x), y - x \rangle \geq 0, \quad \forall y \in M \tag{1.79}$$

is called a *variational inequality of the first kind*.

For arbitrary operators F and subsets M, the existence of a solution $x \in M$ which satisfies the variational inequality (1.79), is not guaranteed. However, in a finite-dimensional setting, Brouwers fixed-point theorem can be applied if the compactness and continuity requirements are met.

Theorem 1.4.1 (Existence of solutions in finite dimensions). *Let $M \subset \mathbb{R}^n$ be a compact and convex set and $F : M \to \mathbb{R}^n$ a continuous function. Then there exists an $\bar{x} \in M$ which satisfies* (1.79).

In order to verify the existence of solutions in infinite dimensions, we make some additional assumptions on the operator F. More precisely, we suppose that F is linear such that the variational inequality can be written as

$$\langle A\bar{x} - f, y - \bar{x} \rangle \geq 0, \quad \forall y \in M, \tag{1.80}$$

where A possesses certain properties introduced below.

Definition 1.4.1 (coercivity, boundedness, symmetry). *A bilinear form $a : H \times H \to \mathbb{R}$ is called coercive if*

$$\exists \xi > 0, \quad \forall y \in H : a(y,y) \geq \xi \, \|y\|_H^2 . \tag{1.81}$$

It is called bounded if

$$\exists \eta > 0, \, \forall y, z \in H : a(y,z) \leq \eta \, \|y\|_H \, \|z\|_H . \tag{1.82}$$

It is called symmetric if

$$\forall y, z \in H : a(z,y) = a(y,z). \tag{1.83}$$

A bounded bilinear form a is always continuous and uniquely determines a linear operator $A : H \to H^*$ via

$$\langle Ax, y \rangle = a(x,y), \quad \forall x,y \in H, \tag{1.84}$$

which naturally inherits the properties - continuity, boundedness and coercivity - of a. The following theorem ensures the existence and uniqueness of solutions to the variational inequality (1.80), cf. [133].

Theorem 1.4.2 (Lion-Stampacchia theorem). *Let $M \subset H$ be non-empty, closed and convex, $a : H \times H \to \mathbb{R}$ a bounded coercive bilinear form and $f \in H^*$. Then there exists a unique $\bar{x} \in M$ which solves the variational inequality*

$$a(\bar{x}, y - \bar{x}) - \langle f, y - \bar{x} \rangle \geq 0, \quad \forall y \in M. \tag{1.85}$$

Additionally, the mapping $f \mapsto \bar{x}$, which assigns to any $f \in H^*$ the solution $\bar{x} \in M \subset H$ of the corresponding variational inequality (1.85)*, is Lipschitz continuous.*

If a is additionally symmetric, (1.85) translates to the necessary and sufficient optimality condition of the convex optimization problem

$$\min_{x \in M} \frac{1}{2} a(x,x) - \langle f, x \rangle. \tag{1.86}$$

Thus, the existence of solutions to (1.85) follows directly from Theorem 1.3.1. Furthermore, the Lipschitz continuity of the mapping $f \mapsto \bar{x}$ can be easily deduced from the coercivity of a.

Although the solution mapping is Lipschitz continuous and therefore directionally differentiable, it is in general not Gateaux differentiable.

The penalization approach

In this section, we briefly introduce a powerful constructive method to solve variational inequalities and optimization problems. The penalization approach allows us to approximate the solutions of these problems by solving a family of non-linear equations or unconstrained optimization problems.

The main idea is to omit the hard restriction to the set M in favor of a penalization of the points outside of M, e.g. by an increase in the objective function. The influence of the corresponding penalty term is then increased by multiplying it with a so-called penalty parameter. For a more detailed explanation of the technique we refer the reader to, e.g., [85, 133, 183].

In case of the optimization problem (1.36), this leads to the following *penalized problem*

$$\min_{x \in X} f(x) + \gamma p(x). \tag{1.87}$$

including the non-negative continuous penalty function $p : X \to \mathbb{R}$ with $ker(p) := \{x \in X \mid p(x) = 0\} = M$ and the *penalty parameter* $\gamma > 0$, which typically goes to infinity. Clearly, if a solution x_γ of the unconstrained problem (1.87) is contained in M, then it also solves the original problem (1.36), since

$$f(x_\gamma) \leq f(x_\gamma) + \gamma p(x_\gamma) \leq f(x) + \gamma p(x) = f(x), \quad \forall x \in M. \tag{1.88}$$

Unfortunately, $\bar{x}_\gamma$ is usually not contained in M. However, the subsequent theorem is easily verified (see e.g. [167]).

Theorem 1.4.3. *Let $f : X \to \mathbb{R}$ be continuous and $\{x_\gamma\}$ be the solutions of* (1.87) *for a sequence $\gamma \to \infty$. Then every accumulation point of $\{x_\gamma\}$ solves the original problem* (1.36).

Applied to the general variational inequality (1.80) the penalty method leads to a family of non-linear equations of the type

$$Ay - f + \gamma\beta(y) = 0, \tag{1.89}$$

where the penalty operator $\beta : H \to H^*$ usually possesses the following properties

1. $ker(\beta) = M$;
2. β is Lipschitz continuous;
3. β is monotone.

Note that (1.89) can be linked to the penalty method for the optimization problem (1.86), if we set $\beta(y) = Dp(y)$.

Using the continuity, coercivity and monotonicity of A and β, it is straightforward to verify the existence of a (unique) solution to (1.89).

Furthermore, the subsequent theorem ensures that the solutions of (1.89) indeed approximate the solution of the variational inequality (1.80) if γ tends to infinity, cf. e.g. [85].

Theorem 1.4.4. *Let $y_\gamma \in H$ solve equation* (1.89) *for a sequence $\gamma \to \infty$. Then the sequence $\{y_\gamma\}$ converges to a point $y \in H$, which satisfies*

$$\langle Ay, v - y \rangle \geq \langle f, v - y \rangle, \quad \forall v \in M. \tag{1.90}$$

The penalization method along with a careful analysis of the limiting properties of the emerging penalized systems forms the foundation for the derivation of stationarity conditions in Chapter 4.

1.5 Semismooth Newton method

Due to their nonsmooth structure, variational inequalities impose various challenges regarding the computation of numerical solutions. In this section we explore a powerful solution method for variational inequalities in infinite dimensional spaces, which is applied in Section 5.2. It relies on a generalized differentiability concept. Some additional information on the subject can be found e.g. in [99, 109, 116, 164]. As above, we consider Banach spaces X, Y and an open subset $M \subset X$.

Definition 1.5.1 (Newton derivative)**.** *The function $f : M \to Y$ is called Newton differentiable on a neighborhood $O \subset M$, if there exists a family of mappings $G : O \to \mathscr{L}(X,Y)$ satisfying*

$$\lim_{h \to 0} \frac{\|f(x+h) - f(x) - G(x+h)h\|_Y}{\|h\|_X} \tag{1.91}$$

for every $x \in O$.

In contrast to more classical differentiability concepts, the derivative is evaluated at the point $x+h$. As a consequence, the Newton derivative is not necessarily unique. However, if f is Fréchet differentiable, then the Newton derivative is unique and both derivatives coincide.

Employing the above definition, we consider the subsequent conceptual Algorithm 1 for solving the equation

$$f(x) = 0. \tag{1.92}$$

Data: $x_0, \varepsilon_{tol} > 0, k := 0$
repeat
    Solve $G(x_k)d_k = -f(x_k)$;
    Set $x_{k+1} := x_k + d_k$ and $k := k+1$;
until $\|f(x)\|_Y < \varepsilon_{tol}$;

Algorithm 1: Semismooth Newton algorithm

If the Newton derivative G is invertible, the iterates x_k produced by Algorithm 1 are well-defined. Furthermore, the following local convergence result can be established, see [109].

Theorem 1.5.1 (Convergence of the semismooth Newton method)**.** *Let $\bar{x}$ be a solution of equation* (1.92) *such that f is Newton differentiable in an open neighborhood $\bar{x} \in O$. Suppose that the Newton derivative $G(x)$ is non-singular for every $x \in O$ and the set $\{\|G^{-1}(x)\| : x \in O\}$ is bounded.*

If the initial point x_0 is sufficiently close to $\bar{x}$, then the iterates x_k generated by Algorithm (1) *converge superlinearly to $\bar{x}$.*

Next, we briefly outline the application of the semismooth Newton method to a variational inequality of the form (1.80). For an open domain $\Omega \subset \mathbb{R}^n$, we consider the problem

$$\langle A\bar{y} - f, y - \bar{y} \rangle \geq 0, \quad \forall y \in M := \{\hat{y} \in L^2(\Omega) : \hat{y} \geq \psi \text{ a.e. on } \Omega\}, \tag{1.93}$$

where $f, \psi \in L^q(\Omega),\ \psi \geq 0, q > 2$ are given and $A \in \mathscr{L}(L^2(\Omega))$ is a self-adjoint coercive operator, which has the following form

$$Ay = Cy + \zeta y, \tag{1.94}$$

with $\zeta > 0$ and $C \in \mathscr{L}(L^2(\Omega), L^q(\Omega))$. By testing (1.93) with $y = 2\bar{y} - \psi$ and $y = \frac{\bar{y}+\psi}{2}$, we observe that the variational inequality is equivalent to the complementarity problem

$$\langle A\bar{y} - f, \bar{y} - \psi \rangle = 0, \qquad \text{a.e. on } \Omega, \tag{1.95}$$

$$\bar{y} - \psi \geq 0, \qquad \text{a.e. on } \Omega, \tag{1.96}$$

$$A\bar{y} - f \geq 0, \qquad \text{a.e. on } \Omega. \tag{1.97}$$

The complementarity can be further reformulated with the help of a so-called NCP-function $\mathscr{C} : L^2(\Omega) \times L^2(\Omega) \to L^2(\Omega)$ such as for instance

$$\mathscr{C}(y_1, y_2) := y_2 - \max(0, y_2 - C(y_1 - \psi)), \tag{1.98}$$

where the max-operator is understood pointwise almost everywhere and C is a positive constant. This leads to the system

$$A\bar{y} - f = \lambda, \text{ a.e. on } \Omega, \tag{1.99}$$

$$\mathscr{C}(\bar{y}, \lambda) = 0, \text{ a.e. on } \Omega. \tag{1.100}$$

Although $\mathscr{C}$ is in general not Fréchet differentiable, it can be shown that it possesses a Newton derivative for certain combinations of domain and images spaces. The proof is based on the following theorem presented by Hintermüller, Ito and Kunish in [109].

Theorem 1.5.2. *The pointwise maximum operator $f_{\max} : L^{p_1}(\Omega) \to L^{p_2}(\Omega)$ with $1 \leq p_2 < p_1 \leq \infty$ given by*

$$[f_{\max}(y)](x) := \max(0, y(x)) = \begin{cases} 0 & \text{if } y(x) \leq 0 \\ y(x) & \text{if } y(x) > 0 \end{cases}, \tag{1.101}$$

is Newton differentiable and an associated Newton derivative is defined by

$$[G(y)](x) := \begin{cases} 0 & \text{if } y(x) \leq 0 \\ 1 & \text{if } y(x) > 0 \end{cases}. \tag{1.102}$$

Due to the above theorem, the problem (1.99)-(1.100) can be solved by the semismooth Newton method. Moreover, the semismooth Newton method coincides with the following primal-dual active set strategy and converges superlinearly if the initial data is sufficiently close to the solution.

Data: Choose $y^0, \lambda^0 \in L^2(\Omega)$. Set $k := 0$.

1 Set $A_k := \{\omega \in \Omega | \lambda^k(\omega) + \beta(y^k(\omega) - \psi(\omega)) > 0\}$ and $I_k := \Omega - A_k$;

2 Solve the system

$$\begin{aligned} Ay^{k+1} + \lambda^{k+1} - f &= 0, \\ y^{k+1} - \psi &= 0 \text{ a.e. on } A_k, \\ \lambda^{k+1} &= 0 \text{ a.e. on } I_k. \end{aligned}$$

3 Stop or set $k := k+1$ and return to line 2.

Algorithm 2: Primal-dual active set strategy

Since the semismooth Newton method and the corresponding convergence analysis were developed in a function space setting, the numerical algorithm and the resulting convergence rates are mesh independent.

1.6 Mathematical programs with equilibrium constraints

A central part of this work is to analyse the challenges connected with the optimal control of specific variational inequalities. In these problems, the state of a system which is influenced by a given control is determined via a variational inequality or complementarity problem. Thus, they fall into the class of so-called mathematical programs with equilibrium constraints (MPECs), where the feasible set is essentially described by an equilibrium condition.

If the variational inequality arises as a necessary first-order condition of an optimization problem itself (cf. Section 1.4), we refer to this problem as the lower-level problem of the MPEC. In this case, the MPEC belongs to the class of bilevel programs, which is a subclass of the so called multilevel programs.

The specific structure of the feasible set imposes several new analytical and numerical challenges which can not be overcome with the classical methods from optimization theory only, see e.g. [143, 168, 169]. Subsequently, we briefly discuss these difficulties and introduce some related mathematical concepts in the context of the following finite dimensional MPEC

$$\begin{aligned} &\min J(z) \\ &s.t.\ \min\{F_{i1}(z),..,F_{il}(z)\} = 0,\ i = 1,..,m, \\ &\qquad g(z) \leq 0,\ h(z) = 0, \end{aligned} \tag{1.103}$$

where $J : \mathbb{R}^n \to \mathbb{R}$, $g : \mathbb{R}^n \to \mathbb{R}^q$, $h : \mathbb{R}^n \to \mathbb{R}^p$ and $F_{ij} : \mathbb{R}^n \to \mathbb{R}$ for $i = 1,..,m$, $j = 1,..,l$ are given functions on $\mathbb{R}^n$.

Note that the constraint system of the MPEC (1.103) constitutes a generalized form of a complementarity system. Moreover, as seen in Section 1.5, variational inequalities can typically be reformulated as such a complementarity system.

If the equality $F_{ij}(z_0) = 0$ holds, we say that the constraint is *active* at z_0. Otherwise, we call it *inactive*. The associated feasible set is given by

$$\mathscr{F}_{MPCC} = \{z : \min\{F_{i1}(z),..,F_{il}(z)\} = 0,\ i = 1,..,m, g(z) \leq 0,\ h(z) = 0\}. \tag{1.104}$$

Moreover, we introduce the corresponding Lagrangian

$$L(\alpha, z, \Lambda, \mu, \lambda) := \alpha J(z) - \sum_{i=1}^{m} \sum_{j=1}^{l} \Lambda_{ij} F_{ij}(z) + \sum_{i=1}^{q} \mu_i g_i(z) + \sum_{i=1}^{p} \lambda_i h_i(z). \tag{1.105}$$

A rather simple way to characterize locally optimal points of the problem (1.103) is based on the Bouligand derivative and the contingent cone defined in (1.41), cf. [143].

Definition 1.6.1 (B-stationarity). *We say that a point $\bar{x} \in \mathscr{F}_{MPCC}$ is B-stationary or Bouligand-stationary, if it satisfies*

$$DJ(\bar{x})h \geq 0, \quad \forall h \in T_{\mathscr{F}_{MPCC}}(\bar{x}). \tag{1.106}$$

Clearly, (1.106) represents a necessary optimality condition for the MPEC (1.103). Nevertheless, it is unclear how to further specify the contingent cone $T_{\mathscr{F}_{MPCC}}(\bar{x})$ at a given point $\bar{x} \in \mathscr{F}_{MPCC}$, which makes the primal stationarity concept (1.106) less usable for practical applications.

In classical optimization theory, we usually argue that the contingent cone has a suitable polyhedral convex form if the problem satisfies a constraint qualification, such as, e.g., (1.66). This allows for the derivation of more explicit multiplier-based stationarity concepts. However, the problem (1.103) normally fails to satisfy any of the classical constraint qualifications, since the corresponding contingent cone is in general neither convex nor polyhedral, due to the structural nonconvexity of the feasible set $\mathscr{F}_{MPCC}$. Thus, we have to acknowledge the combinatorial nature of the complementarity constraints, which leads to a variety of different stationarity concepts.

Using Clarke's stationarity conditions for programs with locally Lipschitzian functions we can establish the existence of nonvanishing multipliers $(\alpha, \hat{\Lambda}, \mu, \lambda)$ with $\alpha \geq 0,\ \lambda \geq 0,\ g(z_0)^T \lambda = 0$ such that

$$0 = \alpha \nabla J(z_0) - \sum_{i=1}^{m} \hat{\Lambda}_i \zeta_i + \sum_{i=1}^{q} \mu_i \nabla g_i(z_0) + \sum_{i=1}^{p} \lambda_i \nabla h_i(z_0), \tag{1.107}$$

where z_0 is an arbitrary local solution of (1.103) and ζ_i is an element of the subdifferential of $\min\{F_{i1}(z_0), .., F_{il}(z_0)\}$, see, e.g., [48, 70]. Since the respective subdifferential can be represented as the convex hull of the gradients $\nabla F_{ij}(z_0)$ of the active constraints at z_0, this gives rise to the following Fritz John type conditions, cf. [169],

$$\alpha \nabla f(z_0) - \sum \Lambda_{ij} \nabla F_{ij}(z_0) + \sum \lambda_i \nabla g_i(z_0) + \sum \mu_i h_i(z_0) = 0, \tag{1.108}$$

$$\alpha \geq 0, \tag{1.109}$$

$$\lambda \geq 0,\ g(z_0)^T \lambda = 0, \tag{1.110}$$

$$F_{ij}(z_0)\Lambda_{ij} = 0,\ \forall i = 1, .., k,\ j = 1, .., m, \tag{1.111}$$

$$\Lambda_{ij}\Lambda_{ir} \geq 0,\ \forall (j, r) : F_{ij}(z_0) = F_{ir}(z_0) = 0. \tag{1.112}$$

We shall see below that the degenerate case $\alpha = 0$ can be excluded if the MPCC satisfies a certain constraint qualification, which leads to the following dual stationarity conditions.

Definition 1.6.2 (C-stationarity)**.** *We call z_0 C-stationary or Clarke stationary if there exist multipliers $\Lambda \in \mathbb{R}^{m\times l}, \lambda \in \mathbb{R}^q, \mu \in \mathbb{R}^p$ such that*

$$\nabla f(z_0) - \sum \Lambda_{ij} \nabla F_{ij}(z_0) + \sum \lambda_i \nabla g_i(z_0) + \sum \mu_i h_i(z_0) = 0, \tag{1.113}$$

$$\lambda \geq 0,\ g(z_0)^T \lambda = 0, \tag{1.114}$$

$$F_{ij}(z_0)\Lambda_{ij} = 0,\ \forall i = 1,..,k,\ j = 1,..,m, \tag{1.115}$$

$$\Lambda_{ij}\Lambda_{ir} \geq 0,\ \forall (j,r) : F_{ij}(z_0) = F_{ir}(z_0) = 0. \tag{1.116}$$

In [168], Scheel presented a different approach relying on a local decomposition of the problem. For a feasible point z_0, we consider an arbitrary collection of active indices

$$\mathscr{A} \subset \left\{(i,j) : F_{ij} = 0\right\}, \tag{1.117}$$

such that for every $i \in \{1,..,m\}$ there exists a $j \in \{1,..,l\}$ with $(i,j) \in \mathscr{A}$. Then we formulate the corresponding ordinary nonlinear program (NLP)

$$\begin{aligned} &\min J(z) \\ &\ s.t.\ F_{ij}(z) = 0,\ \text{if } (i,j) \in \mathscr{A},\quad F_{ij}(z) \geq 0 \text{ otherwise}, \\ &\qquad g(z) \leq 0,\ h(z) = 0, \end{aligned} \tag{1.118}$$

where we set F_{ij} equal to zero for all indices in $\mathscr{A}$. Note that every point $z \in \mathbb{R}^n$ contained in the feasible set

$$\begin{aligned} \mathscr{F}_{\mathscr{A}} = \{z : F_{ij}(z) = 0,\ &\text{if } (i,j) \in \mathscr{A}, F_{ij}(z) \geq 0 \text{ otherwise}, \\ &g(z) \leq 0,\ h(z) = 0\}. \end{aligned} \tag{1.119}$$

satisfies $F_{ij}(z) \geq 0$ for every pair (i,j) of indices and therefore

$$\min\{F_{i1}(z),..,F_{il}(z)\} = 0,\ \forall 1 \leq i \leq m, \tag{1.120}$$

due to the definition of $\mathscr{A}$. Hence $\mathscr{F}_{\mathscr{A}}$ is contained in $\mathscr{F}_{MPCC}$. Furthermore, the Lagrange functions of both optimization problems coincide for every possible choice of $\mathscr{A}$.

For the special case, where we enforce equality to zero on all active indices, i.e. $\mathscr{A} = \left\{(i,j) : F_{ij} = 0\right\}$, the NLP is called the tightened NLP (TNLP) with respect to z_0 associated with (1.103)

$$\begin{aligned} &\min J(z) \\ &\ s.t.\ F_{ij}(z) = 0,\ \text{if } F_{ij}(z_0) = 0 \\ &\qquad F_{ij}(z) \geq 0,\ \text{if } F_{ij}(z_0) > 0 \\ &\qquad g(z) \leq 0,\ h(z) = 0. \end{aligned} \tag{1.121}$$

In addition, we introduce the so-called relaxed NLP (RNLP) with respect to z_0

$$\begin{aligned}
&\min J(z)\\
&s.t.\ F_{ij}(z)=0,\ \text{if } F_{ir}(z_0)>0 \text{ for every } r\neq j\\
&\qquad F_{ij}(z)\geq 0 \text{ otherwise},\\
&\qquad g(z)\leq 0,\ h(z)=0,
\end{aligned} \tag{1.122}$$

which enforces equality to zero only if there is exactly one active constraint.

These nonlinear programs 'encase' the MPCC (1.103) in the following sense. Since every inactive constraint remains inactive in a sufficiently small neighborhood O of z_0, i.e.

$$F_{ij}(z_0)>0 \Rightarrow \exists O \ni z_0\ \forall z\in O\ :\ F_{ij}(z)>0, \tag{1.123}$$

the associated feasible sets locally obey the following chain of inclusions

$$\mathscr{F}_{TNLP}=\bigcap_{\mathscr{A}}\mathscr{F}_{\mathscr{A}}\subset \mathscr{F}_{MPCC}=\bigcup_{\mathscr{A}}\mathscr{F}_{\mathscr{A}}\subset \mathscr{F}_{RNLP},$$

where we intersect and union over all possible choices of $\mathscr{A}$, cf. [169]. Consequently, a local minimizer of the relaxed NLP (1.122) is also a local minimizer of the MPEC (1.103) and a local minimizer of (1.103) is always a local minimizer of the tightened NLP (1.121). Moreover, z is a local minimizer of (1.103) if and only if it locally optimizes the associated nonlinear programs for every possible choice of $\mathscr{A}$.

This motivates us to define the following weak and strong stationarity conditions for the problem (1.103), which are equivalent to the Karush-Kuhn-Tucker conditions of the TNLP and the RNLP, respectively.

Definition 1.6.3 (Weak and strong stationarity)**.** *We refer to z_0 as a weakly stationary point if there exist multipliers $\Lambda\in\mathbb{R}^{m\times l},\lambda\in\mathbb{R}^q,\mu\in\mathbb{R}^p$ such that*

$$\nabla f(z_0)-\sum\Lambda_{ij}\nabla F_{ij}(z_0)+\sum\lambda_i\nabla g_i(z_0)+\sum\mu_i h_i(z_0)=0, \tag{1.124}$$

$$\lambda\geq 0,\ g(z_0)^T\lambda=0, \tag{1.125}$$

$$F_{ij}(z_0)\Lambda_{ij}=0,\ \forall i=1,..,k,\ j=1,..,m. \tag{1.126}$$

We call z_0 S-stationary or strongly stationary if there exist unique multipliers $\Lambda\in\mathbb{R}^{m\times l},\lambda\in\mathbb{R}^q,\mu\in\mathbb{R}^p$ satisfying the system (1.124)-(1.126) *and*

$$\Lambda_{ij}\geq 0,\ \forall j:\exists r\ F_{ij}(z_0)=F_{ir}(z_0)=0. \tag{1.127}$$

Due to the above observations, we immediately deduce that any optimal point z_0 of (1.103) has to satisfy the first-order optimality conditions of the TNLP and is therefore weakly stationary. However, the weak stationarity system (1.124)-(1.126) contains no information on the multiplier Λ_{ij} if the constraint is active, i.e. $F_{ij}(z_0) = 0$. In [169], Scheel and Scholtes have proven the subsequent theorem providing more restrictive characterizations of locally optimal points. Here, we declare that the MPCC (1.103) satisfies the LICQ, MFCQ, or SMFCQ at z_0, if the associated TNLP satisfies the respective constraint qualification for nonlinear programs at z_0, cf. Section 1.3.

Theorem 1.6.1. *Let z_0 be a locally optimal point of the MPCC* (1.103).

(I) If MFCQ holds at z_0, then z_0 is C-stationary.

(II) If SMFCQ holds at z_0, then z_0 is a strongly stationary point.

For a better illustration of these stationarity concepts, we consider the two dimensional MPCC

$$\min_{(z_1,z_2)\in\mathbb{R}^2} J(z_1,z_2) \quad s.t. \ \min\{z_1,z_2\} = 0. \tag{1.128}$$

The feasible set

$$\mathscr{F} = \{(z_1,z_2) \in \mathbb{R}^2 : \min\{z_1,z_2\} = 0\} \tag{1.129}$$

of the MPCC (1.128) corresponds to the positive parts of the coordinate axes and coincides with the contingent cone of the feasible set at the point $\hat{z} = (0,0)$, cf. Figure 1.1. It can be seen that the feasible set is non-smooth, non-convex and does not possess any inner points.

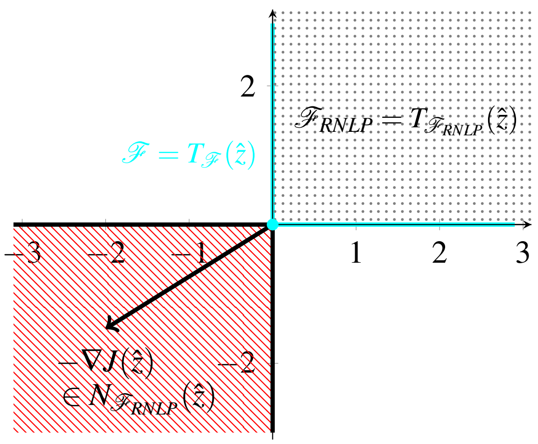

Figure 1.1: Illustration of the stationarity concepts for the MPCC (1.128).

We observe that $\hat{z}$ is a locally optimal point of the MPCC if and only if the negative gradient $-\nabla J(\hat{z})$ points into the red area. This corresponds to

$$-\nabla J(\hat{z}) \in [T_{\mathscr{F}_{RNLP}}(\hat{z})]^0 = N_{\mathscr{F}_{RNLP}}(\hat{z}), \tag{1.130}$$

where the contingent cone of $\mathscr{F}_{RNLP}$ at $\hat{z}$ coincides with the feasible set of the associated RNLP at $\hat{z}$ itself. Indeed, since the SMFCQ is satisfied at $\hat{z}$, the strong stationarity system is a necessary condition for the optimality of $\hat{z}$. In other words, the Karush-Kuhn-Tucker conditions of the RNLP have to be fulfilled. In particular, the sign conditions for Λ, i.e. (1.127), are only satisfied if the inclusion (1.130) holds.

In contrast, the TNLP at $\hat{z}$ possesses only one feasible point. Consequently, the less restrictive weak stationarity system holds at $\hat{z}$, regardless of the form of J (e.g. also for $J = -z_1$, where $\hat{z}$ is clearly not a local minimizer).

In this example, C-stationarity relates to the case where $-\nabla J(\hat{z})$ points into any of the highlighted areas, i.e.

$$-\nabla J(\hat{z}) \in T_{\mathscr{F}_{RNLP}}(\hat{z}) \cup N_{\mathscr{F}_{RNLP}}(\hat{z}). \tag{1.131}$$

In general, the stationarity concepts comply with the following scheme, cf. [169]:

S-stationarity $\Rightarrow$ B-stationarity $\Rightarrow$ C-stationarity $\Rightarrow$ weak stationarity.

For the sake of completeness, we also mention the concept of Mordukhovich or M-stationarity, which is based on Mordukhovich's generalized differential constructions and calculus. For more details on M-stationary points we refer the reader to, e.g., [151, 188]

The above discussion provides a basic introduction to the difficulties connected with the derivation of necessary optimality conditions for MPECs and the associated stationarity concepts. In the course of this thesis, we further elaborate on these topics in the context of infinite dimensional optimal control problems, see e.g. Section 3.3.

1.7 Finite elements

In this work, we occasionally employ adaptive finite elements to compute solutions of various partial differential equations or variational problems. The finite element method is a numerical technique to approximate continuous quantities by discrete nodal values. Since it relies on local approximations, it usually produces sparse equation systems for the discretized problem which decreases the computation time.

For a Hilbert space H, a bilinear form $a : H \times H \to \mathbb{R}$ and $f \in H^*$ we consider the problem of finding $\bar{x} \in H$ such that the equation

$$a(\bar{x}, y) = \langle f, y \rangle, \quad \forall y \in H \tag{1.132}$$

is satisfied. If the bilinear form a is coercive and bounded, equation (1.132) has a unique solution due to the Lax-Milgram theorem.

Following the Galerkin approach, we solve (1.132) in the (finite dimensional) space H_h instead, i.e. we look for an element $\bar{x}_h \in H_h$ which satisfies

$$a(\bar{x}_h, y) = \langle f, y \rangle, \quad \forall y \in H_h. \tag{1.133}$$

Note that the discrete problem (1.133) adopts many properties from the original problem such as e.g., the unique solvability of (1.133) by the Lax-Milgram theorem. This is even more so if H_h is a subspace of the infinite dimensional space H, in which case we speak of a conforming finite element method.

Cea's lemma now ensures that a solution $\bar{x}_h$ of (1.133) is the best approximation of the original solution $\bar{x} \in H$ in H_h in the following sense

$$\|\bar{x} - \bar{x}_h\| \leq C \|\bar{x} - y\|, \quad \forall y \in H_h, \tag{1.134}$$

see e.g. [32].

In two dimensions, a prominent example for the discretization of Sobolev spaces, such as, e.g., $L^2(\Omega)$, $H^1(\Omega)$, is the space of continuous, piecewise linear functions on $\Omega \subset \mathbb{R}^2$. It is defined on a regular triangulation

$$\mathscr{T} = \bigcup_{k=1}^{n} T_k = \Omega \tag{1.135}$$

of the polygonal domain Ω. Here, $T_1, .., T_k$ are triangles such that intersections of two different triangles is either the empty set or it is equal to an edge or a node of both triangles. In the following, we denote the set of all edges of a triangle $T \in \mathscr{T}$ by $\mathscr{E}(T)$ and the set of all nodes T by $\mathscr{E}(T)$.

Then the space V_1 of continuous, piecewise linear functions is defined by

$$V_1 := \{ v \in C(\mathscr{T}) \,|\, v|_{T_k} \in P^1(T_k^i), k = 1, \ldots, n \}, \tag{1.136}$$

where $P_i(T)$ denotes the set of all polynomials on T with degree i. Additionally, we introduce the space V_2 of continuous, piecewise quadratic functions

$$V_2 := \{v \in C(\mathscr{T}) \,|\, v|_{\partial\Omega} = 0, v|_{T_k^i} \in P^2(T_k), k = 1, \ldots, n\}. \tag{1.137}$$

Chapter 2

The Cahn–Hilliard–Navier–Stokes system

2.1 Modelling of incompressible two-phase flows with different densities

The interest in the scientific research on two-phase flows and the interface between two fluids in particular started in the beginning of the 19th century. Scientists like Carl Friedrich Gauß, Pierre-Simon Laplace, and Thomas Young thought of the interface between the fluids as a surface with zero thickness which possesses certain physical properties, e.g. a surface tension, and based their research on static or mechanical equilibrium arguments. Thereby, it was presumed that physical quantities are discontinuous across the interface and the respective physical processes were represented by boundary conditions acting on the interface, which led to the formulation of free-boundary problems.

A few decades later, Siméon Denis Poisson and Josiah Willard Gibbs, among others, discussed the idea that the physical quantities instead perform a gradual smooth transition on the interface between the two phases.

The first scholars to attribute a finite width to the interface were John William Strutt and Johannes Diderik van der Waals, who investigated gradient theories for the interface based on thermodynamic principles such as the van der Waals equation of state. Expanding on these investigations, Diederik Johannes Korteweg deduced a constitutive law for the capillary stress tensor T to model the interface between two fluids, which involves the density ρ and the identity tensor I

$$T \propto (\rho \nabla^2 \rho + \frac{1}{2}|\nabla\rho|^2) I - \nabla\rho \otimes \nabla\rho, \tag{2.1}$$

where $\propto$ signifies that the terms are proportional to each other. In this setting, density distinguishes the bulk fluids and the interface in between. More precisely, $\nabla\rho$ becomes zero on the bulk fluids, where ρ is constant. This is why we also refer to ρ as the order parameter of the system.

Although the free-boundary description has been successful for a variety of applications, the diffuse interface approach has two main advantages. If the width of the interface is comparable to the length scale of the phenomena being examined, e.g. the motion of a contact line along a solid surface which requires a precise modelling of the fluid motion in the vicinity of the contact line, the representation of the interface as a boundary of zero thickness may not be adequate. Secondly, the diffuse interface approach naturally incorporates topological changes of the interface, such as the break-up of liquid droplets or the coalescence of interfaces, which lead to serious difficulties, both analytically and numerically, if the interface is described by a moving, possibly self-intersecting boundary.

2.1.1 The Cahn-Hilliard equation

In 1958, John W. Cahn and John E. Hilliard (see [44]) presented their well-known phase-field model for binary fluids undergoing spinodal decomposition under isothermal and isochoric conditions.

In this context, spinodal decomposition denotes the process where two components, which were mixed to form a single substance, rapidly decompose into two coexisting phases. In contrast to nucleation, in which sufficiently large nuclei of one phase appear randomly and grow, spinodal decomposition does not involve a free energy barrier and therefore the whole solution appears to nucleate at once, and periodic or semi-periodic structures can be observed.

The model is based on a generalized mass diffusion equation in terms of the local diffusion mass flux F and an order parameter φ, which represents the composition of the two phases

$$\partial_t \varphi = \mathrm{div} F, \tag{2.2}$$

where the mass flux F satisfies the boundary condition

$$F \cdot \vec{n}_{|\partial\Omega} = 0. \tag{2.3}$$

Following Fick's law, the mass flux is proportional to the gradient of the chemical potential μ

$$F = m(\varphi)\nabla\mu, \tag{2.4}$$

where $m(\varphi) \geq 0$ depicts the non-negative mobility depending on the concentration. Here, the (degenerate) case $m(\varphi) = 0$ corresponds to a pure transport of the components without diffusion. Following the Ginzburg-Landau theory, the chemical potential is defined as the variational derivative of the free energy E

$$E(\varphi) = \int_\Omega \frac{\sigma\varepsilon}{2}|\nabla\varphi|^2 + \frac{\sigma}{\varepsilon}\Psi(\varphi)dx. \tag{2.5}$$

The first term of the right-hand side represents the surface tension of the interface, whereas $\Psi(\varphi)$ originates from the Helmholtz free energy density per molecule of the homogeneous system with composition φ. The parameters σ and ε are related to the interfacial energy, and the thickness of the interfacial region, respectively.

As a result, the Cahn-Hilliard system reads as follows

$$\partial_t \varphi - \mathrm{div}(m(\varphi)\nabla\mu) = 0, \tag{2.6}$$

$$-\frac{\sigma\varepsilon}{2}\Delta\varphi + \frac{\sigma}{\varepsilon}\partial\Psi(\varphi) - \mu = 0, \tag{2.7}$$

which corresponds to the H^{-1}-gradient flow of the Ginzburg-Landau energy in (2.5), cf. [71]. If we instead consider the associated L^2-gradient, we obtain the classical Allen-Cahn equation

$$\partial_t \varphi + m(\varphi)\Big(-\frac{\sigma\varepsilon}{2}\Delta\varphi + \frac{\sigma}{\varepsilon}\partial\Psi(\varphi))\Big) = 0, \tag{2.8}$$

which is often applied in materials science for solid-liquid phase changes, such as crystal growth. The main difference between these phase separation models is that the order parameter φ is not conserved for the Allen-Cahn equation, whereas for the Cahn-Hilliard equation it is.

In the past decades, the Cahn–Hilliard equation has been shown to be a qualitatively meaningful model for various diffusive processes, such as, e.g., growth and dispersal in population or phase transitions in binary alloys or polymer solutions [49, 161, 176, 179].

Free energy density and spinodal decomposition

An important part in modeling the phase separation process is the choice of Ψ. According to Ginzburg and Landau, the free energy can be obtained by integrating a homogeneous free energy density over a given volume fraction. The first term of the Ginzburg-Landau energy (2.5) then emerges from the inclusion of spatial inhomogeneities, which is important in guaranteeing the conservation of the order parameter. The second part is directly related to the free energy density, cf., e.g., [156].

We point out that this is a phenomenological modelling approach and can not be derived from a more microscopic description of the system. As a consequence, the choice of the free energy density can not be uniquely specified.

In their original work, Cahn and Hilliard considered a logarithmic barrier function

$$\Psi_{\ln}(\varphi) = (\ln(\varphi)\varphi + \ln(1-\varphi)(1-\varphi)) - \frac{\kappa}{2}\varphi^2. \tag{2.9}$$

Another important choice is the double-well potential given by

$$\Psi_W(\varphi) = \frac{\kappa}{2}\varphi^2(1-\varphi^2), \tag{2.10}$$

which is considered, e.g., in [31, 163]. A discussion on the inclusion of higher than quadratic order terms and other variants can be found in [177].

However, in [157, 158], Oono and Puri model the phase separation process utilizing cell dynamical systems, which are space-time discrete dynamical systems with a variable defined on each lattice point and updated in discrete time steps. The state of the lattice at a given time step is usually a function of the state at previous time steps

$$\varphi(t+1,n) = \psi(\varphi(t,n)) + D(g(\varphi(t,n)) - \varphi(t,n)), \tag{2.11}$$

where $\varphi(t,n)$ is the value of the order parameter in the cell n at time t, ψ describes the local dynamics of each cell (without any constraints) and D is a positive constant proportional to the phenomenological diffusion constant. Furthermore, g corresponds to the isotropized discrete Laplacian and can be defined by

$$\begin{aligned} g(\varphi(t,n)) =& \frac{1}{6}\sum(\varphi \text{ in the nearest-neighbor cells}) \\ &+ \frac{1}{12}\sum(\varphi \text{ in the next-nearest-neighbor cells}). \end{aligned} \tag{2.12}$$

The resulting cell dynamical system can be related to the Cahn-Hilliard system (2.6)-(2.7) by utilizing a specific discretization of the partial differential equations.

In this context, the first term of (2.5) reflects the relationship between different molecules or cells, which, e.g., causes the surface tension. In contrast, the second term models the properties of an isolated cell driven by a relaxational mechanism associated to a local free-energy functional.

Comparing different choices for the free energy, Oono and Puri found that short-time simulations based on (2.9) and (2.10) lead to solutions associated to the so-called “soft-wall” regime, in which the thickness of the boundary is appreciable relative to the representative pattern size. In order to obtain “hard-wall” behavior, i.e. sharp domain walls, whose thickness is negligible compared to the pattern size, simulations over a longer time period are necessary. In contrast, for the double-obstacle potential

$$\Psi(\varphi) = i_{[-1,1]}(\varphi) - \frac{\kappa}{2}\varphi^2, \tag{2.13}$$

where $i_{[-1,1]}$ represents the indicator function defined in Section 1.1, the “hard-wall” scenario was observed after very short time spans. This can be related to the fact that for binary alloys without any vacancies, the order parameter should always be contained in the physically relevant interval $[-1,1]$ and this requires vertical potential walls. Furthermore, since the disordered phase is unstable, the functional should be concave on $[-1,1]$. Thus, in many cases, including, e.g., deep quenches of binary alloys or polymeric membrane formation under rapid wall hardening, the double-obstacle potential appears to be the best choice for modelling the phase separation process.

In this thesis, we mainly focus on two-phase flows associated with the double-obstacle potential. However, due to the non-differentiability of the indicator function, the double-obstacle potential leads to the presence of a variational inequality of fourth order in (2.7), cf. Section 1.4. This highly complicates the analytical and numerical treatment of these systems and associated problems, as we will see in the subsequent sections.

Nevertheless, we point out that the potentials (2.9),(2.10),(2.13) share the important characteristics of a single hyperbolic unstable fixed point and two hyperbolic stable fixed points symmetrically placed on each of its sides, corresponding to the disordered state before quenching and the ordered states after quenching, respectively. Therefore, a large number of the cells have order parameter values close to those of the hyperbolic stable fixed points. These cells form the bulk phases. As a consequence, the behavior of the cells near the phase boundaries is governed by the cells in the bulk phases. Thus the global behavior is determined by the hyperbolicity of the sinks, ensuring the structural stability of the model. More precisely, most solutions to the associated Cahn-Hilliard equations that start with initial data near a fixed constant in the spinodal region, i.e., the interval where $\Psi'' < 0$, exhibit fine-grained decomposition. This is called the principle of spinodal decomposition.

The sharp interface limit

As discussed above, the solutions of the Cahn-Hilliard system or the Allen-Cahn equation will form large connected areas of each phase over time. These bulk regions are separated by a small interfacial band in which the order parameter performs a smooth transition from one value (-1 or 1) to the other. In the course of this the regularizing effect of the penalization of the gradient $\nabla\varphi$, i.e. the first term in (2.5), ensures that the order parameter does not make too rapid changes such as jumps. As a consequence, phase field models like the Cahn-Hilliard system and the Allen-Cahn equation can be related to sharp interface models by identifying the boundary surface with the small interfacial layer. Moreover, if the thickness of the interfacial region is driven to zero, the resulting limit systems can be typically linked to sharp interface models. In [150], Modica has shown that the interfacial region, i.e. the set

$$\{x \in \Omega | -1 < \varphi(x) < 1\} \tag{2.14}$$

vanishes almost everywhere, if the interface width ε tends to zero. As a part of that, he additionally proved that the Ginzburg Landau energy in (2.5) Γ-converges in $L^1(\Omega)$ to a multiple of the perimeter functional given by

$$E_{\lim}(\varphi) := \begin{cases} \int_{-1}^{1} \sqrt{2\Psi(y)}dy \int_\Omega |\nabla\chi_{\{\varphi=1\}}(x)|dx & \text{if } \varphi \in BV(\Omega,\{-1,1\}) \\ \infty & \text{if } \varphi \notin BV(\Omega,\{-1,1\}) \end{cases}, \tag{2.15}$$

if ε goes to zero.

Sharp interface models introduce a moving hypersurface $\Gamma(\tau)$ which divides the domain $\Omega \in \mathbb{R}^n$ into two distinct sets $\Omega^+ \subset \Omega$ and $\Omega^- \subset \Omega$. The sets Ω^+ and Ω^- adopt the roles of the sets $\{\omega \in \Omega | \varphi(\omega) = 1\}$ and $\{\omega \in \Omega | \varphi(\omega) = -1\}$, respectively, and describe the different phases. The evolution of Γ is commonly described with the help of a parametrization over a reference manifold $\hat{\Gamma}$.

For a vector field $\mathbf{u} : \hat{\Gamma} \to \mathbb{R}^n$ and a mapping $\mathbf{X}(\tau;\mathbf{u})(\cdot) : \hat{\Gamma} \to \mathbb{R}^n$ we characterize the interface at the time $\tau \geq 0$ by

$$\Gamma(\tau) = \mathbf{X}(\tau;\mathbf{u})(\hat{\Gamma}), \tag{2.16}$$

where the equation is evaluated for each $x \in \hat{\Gamma}$. Possible choices for the base manifold $\hat{\Gamma}$ can be the given surface $\Gamma_0 = \Gamma(0)$ of the initial configuration or a suitable topological object, e.g. a sphere, of the corresponding dimension. Moreover, $\mathbf{u}$ often times relates to a velocity field for the interface motion, e.g.

$$\mathbf{u} = V\nu, \tag{2.17}$$

such that $\mathbf{X}$ is given by

$$\mathbf{X}(\tau;\mathbf{u})(\Gamma_0) = \Gamma_0 + \tau\mathbf{u}(\Gamma_0), \tag{2.18}$$

where '$+$' is understood in the sense that for $x \in \Gamma_0$, $\mathbf{X}(\tau;\mathbf{u})(x) = x + \tau\mathbf{u}(x)$.

One of the most prominent examples is the so-called mean curvature flow. Here, the normal velocity is equal to the mean curvature of the surface, i.e.

$$V = H, \tag{2.19}$$

where the mean curvature H is defined as the sum of the principal curvatures.

The mean curvature flow is approximated by the Allen-Cahn equation (2.8) if ε is driven to zero, see, e.g., [43, 56, 69, 166] for a rigorous interface asymptotics analysis for double-well potentials and [47] for the corresponding convergence result for the double-obstacle potential. More precisely, the Hausdorff distance between the zero-level set of the phase field solution associated to the Allen-Cahn equation and the corresponding surface solution of the mean curvature flow is bounded by the ε, cf. e.g. [24, 45] (double-well potential) and [153] (double-obstacle potential). Moreover, the zero-level set of the phase field solution converges to the viscosity solution of the level-set formulation of the mean curvature flow, see e.g. [69] for the double-well potential and [155] for the double-obstacle potential.

In case of the Cahn-Hilliard system the resulting sharp interface model is the so-called Mullins-Sekerka problem

$$\Delta\mu = 0 \qquad \text{on } \Omega \setminus \Gamma_t, \tag{2.20}$$

$$2V = -[\nabla\mu]_-^+ \cdot \nu \qquad \text{on } \Gamma_t, \tag{2.21}$$

$$2\mu = CH \qquad \text{on } \Gamma_t, \tag{2.22}$$

where $[\nabla\mu]_-^+$ represents the jump of a $\nabla\mu$ across the interface from Ω^+ to Ω^-. In this case, similar convergence results can be derived. For more information on the subject, we refer the reader to, e.g., [12, 46, 161, 178].

2.1.2 Incorporating hydrodynamic effects

An adequate description of the behavior of two-phase flows requires the inclusion of the hydrodynamic effects that occur. A first basic model combining the phase separation process with hydrodynamical properties was given by Pierre Claude Hohenberg and Bertrand I. Halperin in [123]. The so-called 'model H' for two incompressible, viscous Newtonian fluids with matched densities led to the following Cahn-Hilliard-Navier-Stokes system

$$\partial_t\varphi + v\nabla\varphi - \mathrm{div}(m(\varphi)\nabla\mu) = 0, \tag{2.23}$$

$$-\frac{\sigma\varepsilon}{2}\Delta\varphi + \frac{\sigma}{\varepsilon}\partial\Psi(\varphi) - \mu = 0, \tag{2.24}$$

$$\rho\partial_t(v) + \rho\mathrm{div}(v\otimes v) - \mathrm{div}(2\eta(\varphi)\varepsilon(v)) + \nabla\Pi + \sigma\varepsilon\mathrm{div}(\nabla\varphi\otimes\nabla\varphi) = 0, \tag{2.25}$$

$$\mathrm{div} v = 0. \tag{2.26}$$

This model describes the two-phase flow in terms of the order parameter φ, the chemical potential μ and the mean velocity v. Moreover, Π denotes the pressure acting on the system and $\eta(\varphi)$ symbolizes the viscosity of the composition.

The Navier-Stokes equation (2.25) relates the rate of increase of the velocity to the convective term

$$\rho\mathrm{div}(v\otimes v)$$

associated to the transport caused by the fluid motion and the diffusive term

$$-\mathrm{div}(2\eta(\varphi)\varepsilon(v))$$

depicting the inherent spread of the fluids due to, e.g., Brownian motion. It further includes capillary forces due to the surface tension, expressed by

$$\sigma\varepsilon\mathrm{div}(\nabla\varphi\otimes\nabla\varphi).$$

It can be verified that the model is thermodynamically consistent in the sense that it obeys a local dissipation inequality and satisfies the second law of thermodynamics, cf. [94].

However, one of the main limitations of model 'H' is that it is only thermodynamically consistent in situations where both fluids (roughly) have the same density. In [60, 174] it is shown that the model is also consistent in the situation of different densities if the kinetic energy of the fluid is defined by using $\sqrt{\rho}|v|^2$ instead of $\rho|v|^2$, where ρ is the distributed density of the fluid and v is the velocity field. The notion of a distributed density is based on φ and by using the densities of the individual fluid components, a global density field is defined by attaching to every point of the computational domain the density of the fluid.

Following the publication of Hohenberg and Halperin, we have seen different approaches to develop a similar model for the case of non-matched densities. In [141], Lowengrub and Truskinovsky introduce a mass averaged/barycentric velocity and derive a thermodynamically consistent generalization of model H for non-matched densities. Unfortunately, the proposed model involves velocity fields with non-zero divergence. In addition, the fact that pressure enters the Cahn-Hilliard equation further complicates the introduction of suitable discretization schemes.

In contrast, Boyer [36] and Ding [60] considered a volume averaged velocity field which led them to slightly different models, where the solenoidality of the velocity field is guaranteed. However, neither global nor local energy estimates could be derived for these models up to now.

In [6], Abels, Garcke and Grün came up with the following Cahn-Hilliard-Navier-Stokes system

$$\partial_t\varphi + v\nabla\varphi - \operatorname{div}(m(\varphi)\nabla\mu) = 0, \tag{2.27a}$$

$$-\Delta\varphi + \partial\Psi_0(\varphi) - \mu - \kappa\varphi \ni 0, \tag{2.27b}$$

$$\begin{aligned}\partial_t(\rho(\varphi)v) + \operatorname{div}(v\otimes\rho(\varphi)v) - \operatorname{div}(2\eta(\varphi)\varepsilon(v)) + \nabla p&\\ + \operatorname{div}(v\otimes J) - \mu\nabla\varphi &= 0,\end{aligned} \tag{2.27c}$$

$$\operatorname{div} v = 0, \tag{2.27d}$$

$$v_{|\partial\Omega} = 0, \tag{2.27e}$$

$$\partial_n\varphi_{|\partial\Omega} = \partial_n\mu_{|\partial\Omega} = 0, \tag{2.27f}$$

$$(v,\varphi)_{|t=0} = (v_a,\varphi_a). \tag{2.27g}$$

It is based on a volume averaged velocity, which is supposed to hold in the space-time cylinder $\Omega\times(0,\infty)$. Here, the density ρ of the mixture of the fluids depends affinely on the order parameter φ via

$$\rho(\varphi) = \frac{\rho_1+\rho_2}{2} + \frac{\rho_2-\rho_1}{2}\varphi, \tag{2.28}$$

where $0<\rho_1\le\rho_2$ are the given densities of the two fluids under consideration. The relative flux $J := -\frac{\rho_2-\rho_1}{2}m(\varphi)\nabla\mu$ corresponds to the diffusion of the two phases. The initial states are given by v_a and φ_a, and $\kappa>0$ is a positive constant.

The equation (2.27d) ensures that the model is based on divergence-free velocity fields and, at the same time, allows for the verification of global energy estimates as seen below in Section 2.2.1. Furthermore, it reduces to the well-known 'model H' for matched densities, i.e. if $\rho_1 = \rho_2$.

In [6], three variants of this model are proposed that can also handle non-Newtonian fluids or additional particles that are transported across the interface but do not interact with it. Another example for the inclusion of surfactants can be found in [83], where a thermodynamically consistent model for two-phase flow with different densities is proposed that includes additional surface active agents. These particles adhere to the interface, following some advection-diffusion equation and sorption laws. On the interface they lower the surface tension of the interface in a small neighborhood. Thus, this model contains a locally varying surface tension and a partial differential equation on a diffuse interface. The article also contains numerical results based primarily on the results of [64] on the simulation of partial differential equations on evolving interfaces.

Moreover, we note that phase field models can naturally be extended to the situation of multi phase flows with more then two fluid components by using a vector-valued phase field equation, see e.g. [30, 38].

2.1.3 The semi-discrete Cahn–Hilliard–Navier–Stokes system

In this subsection, we introduce a discretization in time of the system (2.27) in its weak formulation, which will be the main subject of our investigations. We start by observing that, assuming integrability in time, from (2.27d), (2.27a), (2.27e), and (2.27f), it follows that the order parameter satisfies

$$\begin{aligned}\int_\Omega \partial_t \varphi dx &= -\int_\Omega v \nabla \varphi dx + \int_\Omega \operatorname{div}(m(\varphi)\nabla\mu) dx \\ &= \int_\Omega \operatorname{div}(v)\varphi dx - \int_{\partial\Omega} v\varphi \vec{n}_\Omega dx + \int_{\partial\Omega} m(\varphi)\nabla\mu \vec{n}_\Omega dx = 0.\end{aligned}$$

In other words, the integral mean of φ remains constant

$$\frac{1}{|\Omega|}\int_\Omega \varphi dx \equiv: \overline{\varphi_a} \in (-1,1), \tag{2.29}$$

which reflects the conservation of mass within the system. Note that the inclusion (2.29) excludes the uninteresting case where only one phase is present, i.e. $|\overline{\varphi_a}| = 1$. This observation allows us to assume that the integral mean of the order parameter is zero without loss of generality, as the general case can easily be transferred to the case $\overline{\varphi_a} = 0$ by considering a shifted system (2.27), where the order parameter is replaced by its projection onto $\overline{L}^2(\Omega)$. This involves a shift in the variables and coefficients such as, e.g. $\Psi_0(\varphi + \overline{\varphi_a})$ and $m(\varphi + \overline{\varphi_a})$, which we again denote by $\Psi_0(\varphi)$ and $m(\varphi)$ (in a slight misuse of notation). Consequently, the two hyperbolic stable fixed points of the free energy describing the pure phases are now associated with the points

$$\psi_1 := -1 - \overline{\varphi_a}, \quad \psi_2 := 1 - \overline{\varphi_a}. \tag{2.30}$$

Our second observation concerns the thermodynamical consistency of the Cahn–Hilliard–Navier–Stokes system. As discussed above, it is possible to derive a (dissipative) energy law for the total energy E consisting of the kinetic energy and the potential energy

$$E(v,\varphi) = \int_\Omega \rho(\varphi)\frac{|v|^2}{2}dx + \int_\Omega \frac{|\nabla\varphi|^2}{2}dx + \Psi(\varphi) \tag{2.31}$$

by testing (2.27a),(2.27b), (2.27c) and (2.27d) with μ, $\partial_t\varphi$, v and Π, respectively, which leads to

$$\partial_t E(v,\varphi) + 2\int_\Omega \eta(\varphi)|\varepsilon(v)|^2 dx + \int_\Omega m(\varphi)|\nabla\mu|^2 dx \leq 0. \tag{2.32}$$

Inequality (2.32) is related to the physical property that the total energy of a closed system is non-increasing and simultaneously serves as a valuable analytical tool, e.g., to secure the boundedness of solutions to (2.27). It is therefore desirable to maintain the energy inequality on the time discrete level, which typically requires preserving the strong coupling of the Cahn–Hilliard system and the Navier–Stokes equation as seen in Definition 2.1.1 below. We note, however, that very recently F. Guillén-González and G. Tierra proposed a numerical splitting scheme for the Cahn–Hilliard–Navier–Stokes system which maintains the energy law via introducing a small correction term to the velocity field, cf. [90].

In order to formulate the mathematical problem we rigorously introduce the given physical data, such as the mobility and viscosity coefficients m,η, the density function ρ, and the initial data v_a,φ_a along with the associated regularity requirements in the following assumption. Note that the subsequent Sobolev spaces are defined in Section 1.2, cf. e.g. (1.19) and (1.27).

Assumption 2.1.1.

(I) The coefficient functions $m,\eta \in C^2(\mathbb{R})$ as well as their derivatives up to second order are bounded, i.e. there exist constants $0 < b_1 \leq b_2$ such that for every $x \in \mathbb{R}$, it holds that $b_1 \leq \min\{m(x),\eta(x)\}$ and

$$\max\{m(x),\eta(x),|m'(x)|,|\eta'(x)|,|m''(x)|,|\eta''(x)|\} \leq b_2. \tag{2.33}$$

(II) The initial state satisfies

$$(v_a, \varphi_a) \in H^2_{0,\sigma}(\Omega;\mathbb{R}^n) \times \left(\overline{H}^2_{\partial_n}(\Omega) \cap \mathbb{K}\right), \tag{2.34}$$

where the constraint set $\mathbb{K}$ *is given by*

$$\mathbb{K} := \left\{\phi \in \overline{H}^1(\Omega) : \psi_1 \leq \phi \leq \psi_2 \text{ a.e. in } \Omega\right\}. \tag{2.35}$$

(III) The density $\rho : \mathbb{R} \to \mathbb{R}$ *depends on the order parameter* φ *via*

$$\rho(\varphi) = \max\left\{\frac{\rho_1 + \rho_2}{2} + \frac{\rho_2 - \rho_1}{2}(\varphi + \overline{\varphi_a}), 0\right\} \geq 0. \tag{2.36}$$

We point out that the Assumption 2.1.1 excludes case of degenerate mobilities, i.e. where $m(\varphi) = 0$. More information on two-phase flows with degenerate mobilities can be found in [5, 66] and, more recently, in [75].

Furthermore, condition (2.36) maintains the (physically given) affine connection of the density ρ to the order parameter φ as long as the order parameter is close to the physically relevant interval $[\psi_1, \psi_2]$. In case of the double-obstacle potential this is always guaranteed by the vertical potential walls at ψ_1 and ψ_2. However, for the double-well potential the order parameter can theoretically attain arbitrary values in $\mathbb{R}$, which requires an artificial extension of the density function onto $\mathbb{R}$. Here, the *max*-operator in (2.36) ensures that the density always remains non-negative, which is important for deriving appropriate energy estimates (see Section 2.2.1).

With these assumptions we present the semi-discrete Cahn–Hilliard Navier–Stokes system. At this point, we additionally introduce a distributed force on the right-hand side of the Navier-Stokes equation, which will later serve the purpose of a distributed control of the system. Note that for actual applications it is natural to consider the control force u_i to be an element of $L^2(\Omega;\mathbb{R}^n)$, in order to permit a point-wise interpretation almost everywhere on Ω.

Moreover, we already include the inherent regularity properties of φ and μ anticipating the results obtained in Lemma 2.2.2. In the following, $\tau > 0$ denotes the time step-size and $M \in \mathbb{N}$ the total number of time instants.

Definition 2.1.1 (Semi-discrete CHNS-system)**.** *Let* $\Psi_0 : \overline{H}^1(\Omega) \to \mathbb{R}$ *be a convex functional with subdifferential* $\partial\Psi_0$. *Fixing* $(\varphi_{-1}, v_0) = (\varphi_a, v_a)$ *we say that a triple*

$$(\varphi, \mu, v) = ((\varphi_i)_{i=0}^{M-1}, (\mu_i)_{i=0}^{M-1}, (v_i)_{i=1}^{M-1})$$

in $\overline{H}^2_{\partial_n}(\Omega)^M \times \overline{H}^2_{\partial_n}(\Omega)^M \times H^1_{0,\sigma}(\Omega;\mathbb{R}^N)^{M-1}$ *solves the semi-discrete CHNS system with respect to a given control* $u = (u_i)_{i=1}^{M-1} \in L^2(\Omega;\mathbb{R}^N)^{M-1}$*, if it holds for all* $\phi \in \overline{H}^1(\Omega)$ *and* $\psi \in H^1_{0,\sigma}(\Omega;\mathbb{R}^N)$ *that*

$$\left\langle \frac{\varphi_{i+1}-\varphi_i}{\tau}, \phi \right\rangle + \langle v_{i+1}\nabla\varphi_i, \phi\rangle + (m(\varphi_i)\nabla\mu_{i+1}, \nabla\phi) = 0, \tag{2.37a}$$

$$(\nabla\varphi_{i+1}, \nabla\phi) + \langle \partial\Psi_0(\varphi_{i+1}), \phi\rangle - \langle \mu_{i+1}, \phi\rangle - \langle \kappa\varphi_i, \phi\rangle \ni 0, \tag{2.37b}$$

$$\begin{aligned}
&\left\langle \frac{\rho(\varphi_i)v_{i+1} - \rho(\varphi_{i-1})v_i}{\tau}, \psi \right\rangle_{H^{-1}_{0,\sigma},H^1_{0,\sigma}} - (v_{i+1}\otimes\rho(\varphi_{i-1})v_i, \nabla\psi) \\
&+ \left(v_{i+1} \otimes \frac{\rho_2-\rho_1}{2} m(\varphi_{i-1})\nabla\mu_i, \nabla\psi \right) + (2\eta(\varphi_i)\varepsilon(v_{i+1}), \varepsilon(\psi)) \\
&\qquad - \langle \mu_{i+1}\nabla\varphi_i, \psi\rangle_{H^{-1}_{0,\sigma},H^1_{0,\sigma}} = \langle u_{i+1}, \psi\rangle_{H^{-1}_{0,\sigma},H^1_{0,\sigma}},
\end{aligned} \tag{2.37c}$$

where the first two equations hold for every $0 \le i+1 \le M-1$ *and the last equation holds for every* $1 \le i+1 \le M-1$.

We denote the associated solution operator by S_Ψ*, i.e.*

$$S_\Psi : u \longmapsto (\varphi, \mu, v). \tag{2.38}$$

Here, the boundary conditions specified in (2.27d)-(2.27f) are incorporated in the respective function spaces of Definition 2.1.1.

We point out that the subdifferential of a convex function Ψ_0 is in general a set-valued mapping, see, e.g., [63]. However, if Ψ_0 is Fréchet differentiable, $\partial\Psi_0$ is single-valued and (2.37b) becomes an equation.

We further note that our semi-discretization of (2.27) in time involves three time instants $(i-1), i, (i+1)$. Equations (2.37a) and (2.37b), however, do not involve the velocity at the time instant $(i-1)$. As a consequence, (φ_0, μ_0) are characterized by the (decoupled) Cahn-Hilliard system only. Nevertheless, the coupling of the Cahn-Hilliard and the Navier-Stokes system is maintained in the subsequent time instances as discussed in the paragraph above. This enables us to verify an energy estimate for the total energy E_i at time step i associated with the semi-discrete system (2.37). Here, the energy functional $E : \overline{H}^1_{0,\sigma}(\Omega) \times \overline{H}^1(\Omega) \times \overline{H}^1(\Omega) \to \mathbb{R}$ is defined by

$$E_i := E(v_i, \varphi_i, \varphi_{i-1}) := \int_\Omega \frac{\rho(\varphi_{i-1})\,|v_i|^2}{2} dx + \int_\Omega \frac{|\nabla\varphi_i|^2}{2} dx + \Psi(\varphi_i), \tag{2.39}$$

where Ψ is given by equation (2.41) below. At this point, we also specify the specific properties of the free energy functionals under consideration. As stated earlier, we focus our research on the double-obstacle potential. However, throughout this thesis, we frequently also discuss free energy densities associated with the double-well potential, see e.g. Section 4.1. More precisely, we study the following two types of free energies.

Assumption 2.1.2. *We suppose that the functional $\Psi_0 : H^1(\Omega) \to \mathbb{R}$ is convex, proper and lower-semicontinuous and possesses one of the two subsequent properties:*

(I) Either it corresponds to the convex part of the double-obstacle potential, i.e.

$$\Psi_0(\varphi) := \int_\Omega i_{[\psi_1,\psi_2]}(\varphi(x))dx; \tag{2.40}$$

(II) Or it originates from a double-well type potential and satisfies:

(a) Ψ_0 is Fréchet differentiable with $\{\Psi_0'(\varphi)\} = \partial\Psi_0(\varphi) \subset L^2(\Omega)$ for every $\varphi \in \overline{H}^1(\Omega)$;

(b) There exists $B_u \in \mathbb{R}$ such that $\Psi_0(\varphi) \leq B_u$ for every $\varphi \in \mathbb{K}$.

Additionally, we assume that the functional

$$\Psi(\varphi) := \Psi_0(\varphi) - \int_\Omega \frac{\kappa}{2}\varphi(x)^2 dx, \tag{2.41}$$

is bounded from below by a constant $B_l \in \mathbb{R}$.

A major goal of this thesis is to study the optimal control of the semi-discrete Cahn–Hilliard–Navier–Stokes system (2.37), where the free energy is related to the double-obstacle potential (2.40). As a first step we discuss the existence of solutions to the Cahn-Hilliard-Navier-Stokes system in the following section.

2.2 Existence of solutions to the Cahn–Hilliard–Navier–Stokes system

When it comes to establishing the existence of solutions to the Cahn–Hilliard–Navier–Stokes system (2.27), the challenges are primarily imposed by the Navier–Stokes equation (2.27c) and, in particular, the non-linear convection term $\mathrm{div}(v \otimes \rho(\varphi)v)$.

In order to address these difficulties, let us consider the simplified problem where the densities and the viscosities of the two phases coincide, i.e.

$$\rho(\varphi) \equiv \rho_1 = \rho_2, \quad \eta(\varphi) \equiv \tilde{\eta}. \tag{2.42}$$

In this case equation (2.27c) reduces to the classical evolutionary non-linear Navier–Stokes equation

$$\partial_t v + \mathrm{div}(v \otimes v) - 2\tilde{\eta}\,\mathrm{div}(\varepsilon(v)) + \nabla\Pi = f_{ext}, \tag{2.43}$$

with the external force $f_{ext} := \mu\nabla\varphi + u$. Here, we briefly recall the proof of existence and uniqueness of weak solutions to the linear Navier–Stokes equation, i.e. without the convection term, which is based on the Faedo-Galerkin method. The problem is approximated using a total sequence $\{\psi_n\}_{n\in\mathbb{N}}$ in $H^1_{0,\sigma}(\Omega)$, i.e. a sequence such that

$$span(\{\psi_1, .., \psi_n, ..\}) \subset H^1_{0,\sigma}(\Omega) \tag{2.44}$$

is dense in $H^1_{0,\sigma}(\Omega)$. A standard fixed point argument ensures that solutions of the auxiliary problems, which are formulated in the subspaces $span(\{\psi_1, .., \psi_n\})$, exist. The solutions are bounded in $L^2(0,T,H^1_{0,\sigma}(\Omega))$ and $L^\infty(0,T,L^2(\Omega))$ and therefore contain a weakly convergent subsequence. Employing (among others) the Rellich-Kondrachov embedding theorem, it can be verified that limit point of the weakly convergent subsequence satisfies equation (2.43) in a distributional sense , cf. [7].

The uniqueness of these solutions can be deduced via an interpolation theorem by Lions-Magenes [138] which yields that the solutions are in fact equivalent to certain continuous functions up to a set of measure zero. Hence, they are contained in $C(0,T,L^2(\Omega))$.

Because of the low regularity of the convection term, these arguments cannot be directly transferred to the non-linear Navier–Stokes equation. Note that the term $(\mathrm{div}(v_1 \otimes v_2), v_3)$ is only well-defined as a trilinear continuous form on $H^1_{0,\sigma}(\Omega) \times H^1_{0,\sigma}(\Omega) \times H^1_{0,\sigma}(\Omega)$ if the space dimension is less than or equal to four. Nevertheless, it can be shown – in addition to the conditions for the linear case –

that the fractional derivatives of some order $0 < \gamma < \frac{1}{4}$ (see Definition 2.2.1) of the sequence of approximate solutions remain bounded in $L^2(\mathbb{R}, L^2(\Omega))$.

Definition 2.2.1. *The fractional derivative $D_t^\gamma f$ of $f : \mathbb{R} \to H$ of order γ is the inverse Fourier transform of $(2i\pi t)^\gamma \mathscr{F}[f](t)$, i.e.*

$$\mathscr{F}[D_t^\gamma f](t) = (2i\pi t)^\gamma \mathscr{F}[f](t), \tag{2.45}$$

where $\mathscr{F}[f]$ represents the Fourier transform of f, cf. Definition 1.2.2.

This enables one to pass to the limit in the convection term which leads to an existence result for weak solutions of the non-linear Navier–Stokes equation, cf. [180].

In two dimensions the uniqueness of these solutions can be shown using the strong embedding properties for two-dimensional Sobolev spaces. This is not the case in higher dimensions due to the insufficient regularity of the velocity field v. Even in three dimensions, there is still a gap between the derived regularity of v ($v \in L^{\frac{8}{3}}(0,T,L^4(\Omega))$ with $\partial_t v \in L^{\frac{4}{3}}(0,T,H^{-1}(\Omega))$) and the regularity requirements for the established uniqueness results (e.g., $v \in L^8(0,T,L^4(\Omega))$) for arbitrary initial data $f_{ext} \in L^2(0,T,H^{-1}(\Omega))$ and $v_a \in L^2(\Omega)$. However, if the initial data is more regular and sufficiently small, uniqueness can also be shown for the three-dimensional case. For arbitrarily large initial data the uniqueness of a weak solution can only be verified on sufficiently small time intervals by choosing a specific spatial basis $\{\psi_n\}_{n\in\mathbb{N}}$.

Another approach to derive the existence of weak solutions to the Navier–Stokes equation is based on an implicit discretization in time and a subsequent limiting analysis with the time step size tending to zero, see e.g., [180]. This falls in line with the research focus of this thesis, namely the analytical and numerical treatment of a semi-discrete Cahn–Hilliard–Navier–Stokes system. In the next subsection, we deduce the existence of solutions to the system (2.37) for single time steps.

2.2.1 The Cahn–Hilliard–Navier–Stokes system for one time step

The goal of this subsection is to establish the existence of solutions to the Cahn–Hilliard–Navier–Stokes system (2.37) for a single time step. More precisely, we ensure the existence of solutions to the slightly generalized system (2.48).

Below, we assume that the following generalized data is given from the previous time step

$$\tilde{\varphi} \in \overline{H}^1(\Omega), \tilde{v} \in H^1_{0,\sigma}(\Omega;\mathbb{R}^N), \nu \in H^1(\Omega;\mathbb{R}^N), f_0, f_{-1} \in L^2(\Omega). \tag{2.46}$$

In case of the double-obstacle potential we additionally assume that

$$\tilde{\varphi} \in \mathbb{K}. \tag{2.47}$$

Definition 2.2.2. *Let $\Psi_0 : \overline{H}^1(\Omega) \to \mathbb{R}$ be a convex functional with subdifferential $\partial\Psi_0$. We say that the triple*

$$(\varphi, \mu, v) \in \overline{H}^1(\Omega) \times \overline{H}^1(\Omega) \times H^1_{0,\sigma}(\Omega;\mathbb{R}^N)$$

solves the generalized Cahn–Hilliard–Navier–Stokes system for one time step for arbitrary right-hand sides $\Theta_v \in (H^1_{0,\sigma}(\Omega;\mathbb{R}^N))^*$ and $\Theta_\mu, \Theta_\varphi \in \overline{H}^{-1}(\Omega)$, if it satisfies

$$\left\langle \frac{\varphi - \tilde{\varphi}}{\tau}, \phi \right\rangle + \langle v\nabla\tilde{\varphi}, \phi\rangle + (m(\tilde{\varphi})\nabla\mu, \nabla\phi) = \langle \Theta_\mu, \phi \rangle, \tag{2.48a}$$

$$-\langle \mu, \phi\rangle - \langle \kappa\tilde{\varphi}, \phi\rangle + (\nabla\varphi, \nabla\phi) + \langle \partial\Psi_0(\varphi), \phi\rangle \ni \langle \Theta_\varphi, \phi\rangle, \tag{2.48b}$$

$$\begin{aligned} \left\langle \frac{f_0 v - f_{-1}\tilde{v}}{\tau}, \psi \right\rangle_{H^{-1}_{0,\sigma}, H^1_{0,\sigma}} &- (v \otimes \nu, \nabla\psi) + (2\eta(\tilde{\varphi})\varepsilon(v), \varepsilon(\psi)) \\ &- \langle \mu\nabla\tilde{\varphi}, \psi\rangle_{H^{-1}_{0,\sigma}, H^1_{0,\sigma}} = \langle \Theta_v, \psi\rangle_{H^{-1}_{0,\sigma}, H^1_{0,\sigma}}, \end{aligned} \tag{2.48c}$$

for every $\phi \in \overline{H}^1(\Omega)$ and every $\psi \in H^1_{0,\sigma}(\Omega;\mathbb{R}^N)$.

Remark 2.2.1. *We point out that the system* (2.48) *corresponds to the system* (2.37) *for one time step if we set*

$$\begin{aligned} &\tilde{v} = v_i,\ \tilde{\varphi} = \varphi_i,\ f_0 = \rho(\varphi_i),\ f_{-1} = \rho(\varphi_{i-1}), \\ &\nu = \rho(\varphi_{i-1})v_i - \frac{\rho_2 - \rho_1}{2} m(\varphi_{i-1})\nabla\mu_i, \\ &\Theta_v = u,\ \Theta_\varphi = \Theta_\mu = 0. \end{aligned} \tag{2.49}$$

However, in Section 4.1 we will encounter a different system of partial differential equations related to the adjoint system of the optimal control problem (3.1.1) introduced below, which can also be shown to possess the form (2.48).

An energy law

Our first objective is to establish a semi-discrete equivalent of the dissipative energy law (2.32) for the solutions of the generalized system (2.48).

Lemma 2.2.1 (Energy estimate for a single time step)**.** *Let $f_0, f_{-1} \geq 0$ and ν satisfy the following equation almost everywhere on Ω*

$$\frac{f_0 - f_{-1}}{\tau} + \operatorname{div}\nu = 0. \tag{2.50}$$

If $(\varphi, \mu, v) \in \overline{H}^1(\Omega) \times \overline{H}^1(\Omega) \times H^1_{0,\sigma}(\Omega; \mathbb{R}^N)$ solves the system (2.48), then the following energy estimate holds true:

$$\begin{aligned}\int_\Omega \frac{f_0 |v|^2}{2} dx + \int_\Omega \frac{|\nabla\varphi|^2}{2} dx + \Psi(\varphi) + \int_\Omega f_{-1} \frac{|v - \tilde{v}|^2}{2} dx + \int_\Omega \frac{|\nabla\varphi - \nabla\tilde{\varphi}|^2}{2} dx \\ + \tau \int_\Omega 2\eta(\tilde{\varphi}) |\varepsilon(v)|^2 dx + \tau \int_\Omega m(\tilde{\varphi}) |\nabla\mu|^2 dx + \int_\Omega \kappa \frac{(\varphi - \tilde{\varphi})^2}{2} \\ \leq \int_\Omega \frac{f_{-1} |\tilde{v}|^2}{2} dx + \int_\Omega \frac{|\nabla\tilde{\varphi}|^2}{2} dx + \Psi(\tilde{\varphi}) + g(\varphi, \mu, v),\end{aligned} \tag{2.51}$$

where g is defined as

$$g(\varphi, \mu, v) := \langle \Theta_\mu, \mu \rangle + \left\langle \Theta_\varphi, \frac{\varphi - \tilde{\varphi}}{\tau} \right\rangle + \langle \Theta_v, v \rangle_{H^{-1}_{0,\sigma}, H^1_{0,\sigma}}. \tag{2.52}$$

Proof. First, we observe that

$$\begin{aligned}(\operatorname{div}(v \otimes \nu), v) &= ((\operatorname{div}\nu)v + (\nu \cdot \nabla)v, v) \\ &= \int_\Omega ((\operatorname{div}\nu)\frac{v}{2} + (\nu \cdot \nabla)v)v dx + \int_\Omega (\operatorname{div}\nu)\frac{v}{2} v dx \\ &= \int_\Omega \operatorname{div}\left(\nu \frac{|v|^2}{2}\right) + (\operatorname{div}\nu)\frac{|v|^2}{2} dx = \int_\Omega (\operatorname{div}\nu)\frac{|v|^2}{2} dx.\end{aligned} \tag{2.53}$$

Next, one verifies

$$\begin{aligned}(f_0 v - f_{-1}\tilde{v}, v) = \int_\Omega \frac{f_0 |v|^2}{2} dx - \int_\Omega \frac{f_{-1} |\tilde{v}|^2}{2} dx \\ + \int_\Omega \frac{(f_0 - f_{-1}) |v|^2}{2} dx + \int_\Omega \frac{f_{-1} |v - \tilde{v}|^2}{2} dx.\end{aligned} \tag{2.54}$$

Testing (2.48a),(2.48b) and (2.48c) with μ, $\frac{\varphi-\tilde{\varphi}}{\tau}$ and v, respectively, and summing up, we obtain

$$0=\int_\Omega \frac{f_0\,|v|^2-f_{-1}\,|\tilde{v}|^2}{2\tau}dx+\int_\Omega f_{-1}\frac{|v-\tilde{v}|^2}{2\tau}dx+\int_\Omega \frac{(f_0-f_{-1})\,|v|^2}{2\tau}dx$$
$$+\int_\Omega (\operatorname{div} v)\frac{|v|^2}{2}dx+\int_\Omega 2\eta(\tilde{\varphi})\,|\varepsilon(v)|^2\,dx+\int_\Omega m(\tilde{\varphi})\,|\nabla\mu|^2\,dx$$
$$+\frac{1}{\tau}\langle\partial\Psi_0(\varphi),\varphi-\tilde{\varphi}\rangle_{\overline{H}^{-1},\overline{H}^1}-\kappa\int_\Omega \tilde{\varphi}\frac{\varphi-\tilde{\varphi}}{\tau}dx$$
$$+\frac{1}{\tau}\int_\Omega \nabla\varphi(\nabla\varphi-\nabla\tilde{\varphi})dx-g(\varphi,\mu,v), \tag{2.55}$$

where we also use the previous equations (2.53) and (2.54). From the definition of the subdifferential we infer

$$\langle\partial\Psi_0(\varphi),\varphi-\tilde{\varphi}\rangle\geq\Psi(\varphi)-\Psi(\tilde{\varphi})+\frac{\kappa}{2}\int_\Omega \varphi^2-\tilde{\varphi}^2dx. \tag{2.56}$$

Additionally, the following equations hold pointwise

$$\nabla\varphi(\nabla\varphi-\nabla\tilde{\varphi})=\frac{|\nabla\varphi|^2}{2}-\frac{|\nabla\tilde{\varphi}|^2}{2}+\frac{|\nabla\varphi-\nabla\tilde{\varphi}|^2}{2} \tag{2.57}$$

and

$$\tilde{\varphi}(\varphi-\tilde{\varphi})=\frac{\varphi^2}{2}-\frac{\tilde{\varphi}^2}{2}-\frac{(\varphi-\tilde{\varphi})^2}{2}. \tag{2.58}$$

Inserting (2.50),(2.56),(2.57) and (2.58) into equation (2.55) proves the assertion. □

With the specific choices of Remark 2.2.1, the total energy E_i at time step i, cf. (2.39), is given by

$$E_i=\int_\Omega \frac{f_{-1}\,|\tilde{v}|^2}{2}dx+\int_\Omega \frac{|\nabla\tilde{\varphi}|^2}{2}dx+\Psi(\tilde{\varphi}). \tag{2.59}$$

Hence, due to the non-negativity of f_0, f_{-1} and the coefficients m, η, all the terms of the left-hand side of the inequality are always non-negative and Lemma 2.2.1 indeed ensures that the energy of the next time step $(i+1)$ is smaller than the sum of E_i and the energy associated with the external force u_{i+1}.

Existence of solutions

The subsequent theorem asserts the existence of solutions to the generalized system (2.48). The proof relies primarily on Schaefer's fixed point theorem (which is also called the Leray-Schauder principle in the literature) and arguments from monotone operator theory. The boundedness condition from Schaefer's fixed point theorem is verified using the energy estimate from Lemma 2.2.1.

Theorem 2.2.1 (Existence of solutions to the CHNS system for a single time step)**.** *Let $f_0, f_{-1} \geq 0$ and ν satisfy equation* (2.50)*.*

Then the system (2.48) *possesses a solution* $(\varphi, \mu, v) \in \overline{H}^1(\Omega) \times \overline{H}^1(\Omega) \times H^1_{0,\sigma}(\Omega; \mathbb{R}^N)$.

Proof. We start by defining

$$X := \overline{H}^1(\Omega) \times \overline{H}^1(\Omega) \times H^1_{0,\sigma}(\Omega; \mathbb{R}^N), \tag{2.60}$$

$$Y := \overline{H}^1(\Omega)^* \times \overline{H}^1(\Omega)^* \times H^1_{0,\sigma}(\Omega; \mathbb{R}^N)^*, \tag{2.61}$$

and the operators $\mathscr{G} : X \rightrightarrows Y$ and $\mathscr{F} : X \to Y$ via

$$\begin{aligned}
\langle \mathscr{G}_1(\mu), \phi \rangle &:= (m(\tilde{\varphi})\nabla\mu, \nabla\phi) - \langle \Theta_\mu, \phi \rangle, \\
\langle \mathscr{G}_2(\varphi), \phi \rangle &:= (\nabla\varphi, \nabla\phi) + \langle \partial\Psi_0(\varphi), \phi \rangle - \langle \Theta_\varphi, \phi \rangle, \\
\langle \mathscr{G}_3(v), \psi \rangle_{H^{-1}_{0,\sigma}, H^1_{0,\sigma}} &:= (2\eta(\tilde{\varphi})\varepsilon(v), \varepsilon(\psi)) - \langle \Theta_v, \psi \rangle_{H^{-1}_{0,\sigma}, H^1_{0,\sigma}}, \\
\mathscr{G}(\varphi, \mu, v) &:= (\mathscr{G}_1(\mu), \mathscr{G}_2(\varphi), \mathscr{G}_3(v))^\top,
\end{aligned}$$

and

$$\begin{aligned}
\mathscr{F}_1(\varphi, \mu, v) &:= -\frac{\varphi - \tilde{\varphi}}{\tau} - v\nabla\tilde{\varphi}, \\
\mathscr{F}_2(\varphi, \mu, v) &:= \mu + \kappa\tilde{\varphi}, \\
\langle \mathscr{F}_3(\varphi, \mu, v), \psi \rangle_{H^{-1}_{0,\sigma}, H^1_{0,\sigma}} &:= \left\langle -\frac{f_0 v - f_{-1}\tilde{v}}{\tau} + \mu\nabla\tilde{\varphi}, \psi \right\rangle_{H^{-1}_{0,\sigma}, H^1_{0,\sigma}} \\
&\quad + (v \otimes \nu, \nabla\psi), \\
\mathscr{F}(\varphi, \mu, v) &:= (\mathscr{F}_1, \mathscr{F}_2, \mathscr{F}_3)^\top.
\end{aligned}$$

Using this notation, the system (2.48) can be stated as

$$0 \in \mathscr{G}(\varphi, \mu, v) - \mathscr{F}(\varphi, \mu, v) \subset Y. \tag{2.62}$$

By standard arguments, the mappings $\mathscr{G}_1$ and $\mathscr{G}_3$ are invertible and the respective inverse mapping is continuous. Since the Laplace operator is invertible from $\overline{H}^1(\Omega)$

to $\overline{H}^1(\Omega)^*$ and the subdifferential $\partial\Psi_0$ is maximal monotone (cf. [165, Theorem A]), $\mathscr{G}_2$ is invertible, as well. Concerning the continuity of $\mathscr{G}_2^{-1}$, let $\xi_1, \xi_2 \in \overline{H}^1(\Omega)^*$ and $\varphi_1, \varphi_2 \in \overline{H}^1(\Omega)$ satisfy $\varphi_j = \mathscr{G}_2^{-1}(\xi_j)$ for $j = 1, 2$. Using Poincaré's inequality and the monotonicity of $\partial\Psi_0$, we immediately obtain

$$\begin{aligned}\|\varphi_2 - \varphi_1\|_{H^1}^2 \leq & C(\nabla(\varphi_2 - \varphi_1), \nabla(\varphi_2 - \varphi_1)) \\ & + C\langle\partial\Psi_0(\varphi_2) - \partial\Psi_0(\varphi_1), \varphi_2 - \varphi_1\rangle \qquad (2.63)\\ = & C\langle\xi_2 - \xi_1, \varphi_2 - \varphi_1\rangle \leq C\|\xi_2 - \xi_1\|_{H^{-1}}\|\varphi_2 - \varphi_1\|_{H^1}, \qquad (2.64)\end{aligned}$$

showing the continuity of $\mathscr{G}_2^{-1}$.

Due to the compact embedding of the space $\overline{Y} := L^{\frac{3}{2}}(\Omega) \times L^{\frac{3}{2}}(\Omega) \times L^{\frac{3}{2}}(\Omega; \mathbb{R}^N)$, into Y, the inverse of $\mathscr{G}$ is a compact operator from $\overline{Y}$ to X. Next, we check that $\mathscr{F}$ is a continuous mapping from X to $\overline{Y}$. Hence, the operator $\mathscr{F} \circ \mathscr{G}^{-1} : \overline{Y} \to \overline{Y}$ is compact.

In what follows, we show the existence of a solution δ^* to the fixed point equation

$$\delta^* - \mathscr{F} \circ \mathscr{G}^{-1}(\delta^*) = 0 \in \overline{Y}. \qquad (2.65)$$

Then it immediately follows that $\mathscr{G}^{-1}(\delta^*)$ solves the system (2.48). In order to apply Schaefer's theorem with respect to the operator $\mathscr{F} \circ \mathscr{G}^{-1}$ we verify the condition that the set $D := \bigcup_{0\leq\lambda\leq 1}\left\{\delta \in \overline{Y} | \delta = \lambda\mathscr{F} \circ \mathscr{G}^{-1}(\delta)\right\}$ is bounded. For this purpose, assume that $\delta \in \overline{Y}$ and $\lambda \in [0, 1]$ satisfy

$$\delta = \lambda\mathscr{F} \circ \mathscr{G}^{-1}(\delta), \qquad (2.66)$$

and define $(\varphi, \mu, v) := \mathscr{G}^{-1}(\delta) \in X$. Thus, (2.66) can be rewritten as

$$\mathscr{G}(\varphi, \mu, v) - \lambda\mathscr{F}(\varphi, \mu, v) = 0 \qquad (2.67)$$

which is equivalent to the following system of equations

$$\begin{aligned}\left\langle\lambda\frac{\varphi - \tilde{\varphi}}{\tau}, \phi\right\rangle + \langle\lambda v\nabla\tilde{\varphi}, \phi\rangle &= -(m(\tilde{\varphi})\nabla\mu, \nabla\phi) + \left\langle\Theta_\mu, \phi\right\rangle, \ \forall\phi \in \overline{H}^1(\Omega),\\ \langle\lambda\mu, \phi\rangle + \langle\lambda\kappa\tilde{\varphi}, \phi\rangle &= (\nabla\varphi, \nabla\phi) + \langle\partial\Psi_0(\varphi)), \phi\rangle - \left\langle\Theta_\varphi, \phi\right\rangle, \ \forall\phi \in \overline{H}^1(\Omega),\\ \lambda\left\langle\frac{f_0 v - f_{-1}\tilde{v}}{\tau}, \psi\right\rangle_{H^{-1}_{0,\sigma}, H^1_{0,\sigma}} & -\lambda(v\otimes v, \nabla\psi) + (2\eta(\tilde{\varphi})\varepsilon(v), \varepsilon(\psi))\\ &= \lambda\langle\mu\nabla\tilde{\varphi}, \psi\rangle_{H^{-1}_{0,\sigma}, H^1_{0,\sigma}} + \langle\Theta_v, \psi\rangle_{H^{-1}_{0,\sigma}, H^1_{0,\sigma}}, \ \forall\psi \in H^1_{0,\sigma}(\Omega; \mathbb{R}^N).\end{aligned}$$

Analogously to the proof of Lemma 2.2.1, we test this system by μ, $\frac{\varphi-\tilde{\varphi}}{\tau}$ and v, and sum up the resulting equations to derive

$$
\begin{aligned}
0 = \lambda \int_\Omega \frac{f_0\,|v|^2 - f_{-1}\,|\tilde{v}|^2}{2\tau} dx + \lambda \int_\Omega f_{-1} \frac{|v-\tilde{v}|^2}{2\tau} dx + \int_\Omega 2\eta(\tilde{\varphi})\,|\varepsilon(v)|^2\,dx \\
+ \int_\Omega m(\tilde{\varphi})\,|\nabla\mu|^2\,dx + \frac{1}{\tau}\langle \partial\Psi_0(\varphi), \varphi-\tilde{\varphi}\rangle - \lambda\kappa \int_\Omega \tilde{\varphi}\frac{\varphi-\tilde{\varphi}}{\tau} dx \\
+ \frac{1}{\tau}\int_\Omega \nabla\varphi(\nabla\varphi - \nabla\tilde{\varphi})dx - g(\varphi,\mu,v),
\end{aligned}
\tag{2.68}
$$

which leads to

$$
\begin{aligned}
&\int_\Omega 2\eta(\tilde{\varphi})\,|\varepsilon(v)|^2\,dx + \int_\Omega m(\tilde{\varphi})\,|\nabla\mu|^2\,dx \\
&\quad + \frac{1}{\tau}\Psi(\varphi) + \frac{1}{\tau}\int_\Omega |\nabla\varphi|^2\,dx - g(\varphi,\mu,v) \\
&\le \lambda \int_\Omega \frac{f_{-1}\,|\tilde{v}|^2}{2\tau} dx + \frac{1}{\tau}\int_\Omega |\nabla\tilde{\varphi}|^2\,dx + \frac{1}{\tau}\Psi(\tilde{\varphi}).
\end{aligned}
\tag{2.69}
$$

Note that for obtaining (2.68) we also make use of (2.50). The right-hand side of (2.69) can be bounded by a constant $C := C(N,\Omega,\tau,f_{-1},\tilde{v},\tilde{\varphi}) > 0$ which is independent of λ. Since Ψ is bounded from below, this leads to

$$
\int_\Omega 2\eta(\tilde{\varphi})\,|\varepsilon(v)|^2\,dx + \int_\Omega m(\tilde{\varphi})\,|\nabla\mu|^2\,dx + \frac{1}{\tau}\int_\Omega |\nabla\varphi|^2\,dx \le C + g(\varphi,\mu,v).
\tag{2.70}
$$

Due to Korn's inequality, Poincaré's inequality and from the boundedness of $\eta(\cdot)$ and $m(\cdot)$, we infer

$$
\begin{aligned}
\|v\|_{H^1}^2 + \|\mu\|_{H^1}^2 + \|\varphi\|_{H^1}^2 &\le C + g(\varphi,\mu,v) \\
&\le C_1 + C_2(\|v\|_{H^1} + \|\mu\|_{H^1} + \|\varphi\|_{H^1}),
\end{aligned}
\tag{2.71}
$$

where $C_2 > 0$ depends only on Θ_μ, Θ_φ and Θ_v. The last inequality yields the boundedness of (φ,μ,v) in X.

Next, we derive bounds for $\mathscr{F}$. In fact, we have

$$
\begin{aligned}
&\|\mathscr{F}_1(\varphi,\mu,v)\|_{L^{3/2}} \le C(\|\varphi\| + \|\tilde{\varphi}\| + \|v\|_{H^1}\,\|\tilde{\varphi}\|_{H^1}), \\
&\|\mathscr{F}_2(\varphi,\mu,v)\|_{L^{3/2}} \le C(\|\mu\| + \|\tilde{\varphi}\|), \\
&\|\mathscr{F}_3(\varphi,\mu,v)\|_{L^{3/2}} \le C(\|v\|_{H^1} + \|v\|_{H^1}\,\|\boldsymbol{\nu}\|_{H^1} + \|\mu\|\,\|\tilde{\varphi}\|_{H^1} + \|\tilde{v}\|_{H^1}).
\end{aligned}
$$

Since $\tilde{\varphi}$, $\tilde{v}$ and $\boldsymbol{\nu}$ are fixed, D is bounded in $\overline{Y}$. Hence Schaefer's theorem is applicable implying that equation (2.65) admits a fixed point $\delta^* \in \overline{Y}$. Then $\mathscr{G}^{-1}(\delta^*)$ solves the system (2.48). $\square$

Regularity of solutions

As noted above, it is possible to derive higher regularity properties for the solution of the Navier–Stokes system if the initial data is sufficiently regular. A similar observation holds true for the solutions of variational inequalities, see, e.g., [133].

Following this line of reasoning it is possible to prove the following lemma via a bootstrap argument if we assume that the right-hand sides of the system (2.48) are square integrable functions.

Lemma 2.2.2 (Regularity of solutions)**.** *Let $\Theta_\mu, \Theta_\varphi \in L^2(\Omega)$, $f_0, f_{-1} \in L^3(\Omega)$, $\tilde{\varphi} \in H^2(\Omega)$ and $v \in H^1(\Omega;\mathbb{R}^N)$ be such that $f_0, f_{-1} \geq 0$ and equation* (2.50) *is satisfied.*

If the triple (φ, μ, v) solves the generalized system (2.48)*, then it holds that*

$$(\varphi,\mu,v) \in \overline{H}^2_{\partial_n}(\Omega) \times \overline{H}^2_{\partial_n}(\Omega) \times H^2_{0,\sigma}(\Omega;\mathbb{R}^N). \tag{2.72}$$

Moreover, there exists a constant $C = C(N,\Omega,b_1,b_2,\tau,\kappa) > 0$ such that

$$\begin{aligned} &\|\varphi\|_{H^2} + \|\mu\|_{H^2} + \|v\|_{H^2} \\ &\qquad \leq C(\|\varphi\| + \|\mu\| + \|\tilde{\varphi}\| + \|\Theta_\varphi\| + \|\Theta_\mu\| + \|v\|_{H^1}\|\tilde{\varphi}\|_{H^2}). \end{aligned} \tag{2.73}$$

In case of the double-obstacle potential, it also holds that $\varphi \in \mathbb{K}$.

Proof. First, we show that φ is an element of the space $\overline{H}^2_{\partial_n}(\Omega)$. We start by considering the case of the double-well type potential and define $g_1 := -(\mu + \kappa\tilde{\varphi} + \Theta_\varphi) + \Psi_0'(\varphi)$. Due to Assumption 2.1.2 (*II*) (a) and Sobolev‘s embedding theorem, g_1 is contained in $L^2(\Omega)$. Then (2.48b) is equivalent to the following equation

$$(\nabla\varphi, \nabla\phi) = \langle g_1, \phi\rangle,\ \forall \phi \in \overline{H}^1(\Omega), \tag{2.74}$$

which has a unique solution $\varphi \in \overline{H}^1(\Omega)$. By [144, Theorem 2.3.6] and [144, Remark 2.3.7], the Neumann problem

$$\Delta\varphi^* = g_1 \text{ a.e. in } \Omega,\ \partial_n\varphi_{|\partial\Omega} = 0 \text{ on } \partial\Omega.$$

has a (unique) solution $\varphi^* \in \overline{H}^2_{\partial_n}(\Omega)$. Here, φ^* is a strong solution and the boundary condition holds true in the trace sense. Consequently, $\varphi = \varphi^* \in \overline{H}^2_{\partial_n}(\Omega)$. Furthermore, [144, Theorem 2.3.1] yields the existence of a constant $C := C(N,\Omega)$ such that

$$\|\varphi\|_{H^2} \leq C(\|\varphi\| + \|g_1\|) \leq C(\|\varphi\| + \|\mu\| + \kappa\|\tilde{\varphi}\| + \|\Theta_\varphi\| + \|\Psi_0'(\varphi)\|). \tag{2.75}$$

In case of the double-obstacle potential, (2.74) is equivalent to the variational inequality problem:

$$\text{Find } \varphi \in \mathbb{K} : \ (\nabla\varphi, \nabla\phi - \nabla\varphi) - \langle g_2, \phi - \varphi \rangle \geq 0, \ \forall \phi \in \mathbb{K} \tag{2.76}$$

with $g_2 := \mu + \kappa\tilde{\varphi} + \Theta_\varphi \in L^2(\Omega)$. Then the assertion follows from the following lemma.

Lemma 2.2.3. *If $\varphi \in \mathbb{K}$ solves the variational inequality problem (2.76) with $g_1 \in L^2(\Omega)$, then $\varphi \in \overline{H}^2_{\partial_n}(\Omega)$ and there exists a constant $C = C(N, \Omega) > 0$ such that*

$$\|\varphi\|_{H^2} \leq C \|g_1\|. \tag{2.77}$$

Proof. Let $L_\varepsilon : \overline{H}^1(\Omega) \to \overline{H}^1(\Omega)^*$ be defined by

$$\begin{aligned} \langle L_\varepsilon(\varphi), \phi \rangle := {} & (\nabla\varphi, \nabla\phi) \\ & - \langle g_2 + \max(-g_2, 0)\theta_\varepsilon(\varphi - \psi_1) + \min(-g_2, 0)\theta_\varepsilon(\psi_2 - \varphi), \phi \rangle \end{aligned} \tag{2.78}$$

where $\phi \in \overline{H}^1(\Omega)$ and θ_ε is defined by

$$\theta_\varepsilon(x) := \begin{cases} 1 & \text{if } x \leq 0, \\ 1 - \frac{x}{\varepsilon} & \text{if } 0 \leq x \leq \varepsilon, \\ 0 & \text{if } x \geq \varepsilon. \end{cases} \tag{2.79}$$

Since $g_2 \in L^2(\Omega)$ and $\theta_\varepsilon(\varphi - \psi_1), \theta_\varepsilon(\psi_2 - \varphi) \in L^\infty(\Omega)$, it holds that

$$\|g_2 + \max(-g_2, 0)\theta_\varepsilon(\varphi - \psi_1) + \min(-g_2, 0)\theta_\varepsilon(\varphi - \psi_2)\| \leq \|g_2\|. \tag{2.80}$$

We show that for every $0 < \varepsilon \leq \min(-\psi_1, \psi_2)$ there exists a unique $\varphi_\varepsilon \in \overline{H}^2_{\partial_n}(\Omega) \cap \mathbb{K}$ such that

$$L_\varepsilon(\varphi_\varepsilon) = 0, \tag{2.81}$$

In fact, for every $w, \phi \in \overline{H}^1(\Omega)$, it can be seen that

$$\begin{aligned} & \langle L_\varepsilon(w) - L_\varepsilon(\phi), w - \phi \rangle \\ & \quad = \langle -\Delta(w - \phi), w - \phi \rangle \\ & \quad - \int_\Omega \max(-g_2, 0) \left(\theta_\varepsilon(w - \psi_1) - \theta_\varepsilon(\phi - \psi_1)\right)(w - \phi) dx \\ & \quad - \int_\Omega \min(-g_2, 0) \left(\theta_\varepsilon(\psi_2 - w) - \theta_\varepsilon(\psi_2 - \phi)\right)(w - \phi) dx \\ & \quad \geq \int_\Omega |\nabla w - \nabla\phi|^2 dx \end{aligned} \tag{2.82}$$

where we use the monotonicity of θ_ε. By Poincaré's inequality there exists a constant $C > 0$ such that

$$\langle L_\varepsilon(w) - L_\varepsilon(\phi), w - \phi \rangle \geq \|\nabla w - \nabla \phi\|^2 \geq C \|w - \phi\|_{H^1}^2 .$$

Consequently, L_ε is strongly monotone and coercive. Since L_ε is also continuous on finite dimensional subspaces of $\overline{H}^1(\Omega)$, [133, III: Corollary 1.8] is applicable which yields the existence of $\varphi_\varepsilon \in \overline{H}^1(\Omega)$ with $L_\varepsilon(\varphi_\varepsilon) = 0$.

With the help of inequality (2.80), we may apply [144, Theorem 2.3.6] and [144, Theorem 2.3.1] similarly to the proof of Lemma 2.2.2 to deduce that $\varphi_\varepsilon \in \overline{H}^2_{\partial_n}(\Omega)$ and there exists a constant $C_1 > 0$ such that

$$\|\varphi_\varepsilon\|_{H^2} \leq C_1 \|\Delta \varphi_\varepsilon\| + \|\varphi_\varepsilon\| . \tag{2.83}$$

In combination with (2.80) and Poincaré's inequality, this leads to

$$\|\varphi_\varepsilon\|_{H^2} \leq C_2 \|g_2\| . \tag{2.84}$$

Now, we set $\beta_\varepsilon := \varphi_\varepsilon - \min(\varphi_\varepsilon, \psi_2) \geq 0$ and observe that

$$\|\nabla \beta_\varepsilon\|^2 = \int_{\Omega_1} \nabla(\varphi_\varepsilon - \psi_2)\nabla \beta_\varepsilon dx = \langle -\Delta \varphi_\varepsilon, \beta_\varepsilon \rangle \tag{2.85}$$

where $\Omega_1 := \{x \in \Omega : \beta_\varepsilon(x) > 0\} = \{x \in \Omega : \varphi_\varepsilon(x) > \psi_2 \geq \psi_1 + \varepsilon\}$. By equation (2.78) and (2.81), this leads to

$$\begin{aligned}
\|\nabla \beta_\varepsilon\|^2 &= \int_{\Omega_1} (g_2 + \max(-g_2, 0)\theta_\varepsilon(\varphi_\varepsilon - \psi_1) \\
&\quad + \min(-g_2, 0)\theta_\varepsilon(\psi_2 - \varphi_\varepsilon))\beta_\varepsilon dx \\
&= \int_{\Omega_1} (g_2 + \min(-g_2, 0))\beta_\varepsilon dx \leq 0.
\end{aligned} \tag{2.86}$$

Thus, $\beta_\varepsilon = 0$ and therefore $\varphi_\varepsilon \leq \psi_2$ almost everywhere in Ω.

In a similar way, we prove that $\varphi_\varepsilon - \max(\varphi_\varepsilon, \psi_1) = 0$ and therefore $\varphi_\varepsilon \geq \psi_1$ almost everywhere on Ω. Hence φ_ε is contained in $\overline{H}^2(\Omega) \cap \mathbb{K}$. By inequality (2.84), the sequence $\{\varphi_\varepsilon\}_{\varepsilon \to 0}$ is bounded in $\overline{H}^2(\Omega)$ and there exists a weakly convergent subsequence (denoted the same) such that $\varphi_\varepsilon \rightharpoonup_{\overline{H}^2} \varphi^*$ with $\|\varphi^*\|_{H^2} \leq C_2 \|g_2\|$. Since $\mathbb{K}$ is weakly closed, it contains φ^*.

For arbitrarily small $0 < \delta \leq \min(-\psi_1, \psi_2)$, let $\phi \in \mathbb{K}$ be such that $\psi_1 + \delta \leq \phi \leq \psi_2 - \delta$ almost everywhere in Ω. Using equation (2.81) and the monotonicity of L_ε, we infer

$$\begin{aligned}
0 \leq \langle L_\varepsilon(\phi), \phi - \varphi_\varepsilon \rangle &= \langle -\Delta \phi, \phi - \varphi_\varepsilon \rangle - \int_\Omega (g_2 + \max(-g_2, 0)\theta_\varepsilon(\phi - \psi_1) \\
&\qquad + \min(-g_2, 0)\theta_\varepsilon(\psi_2 - \phi))(\phi - \varphi_\varepsilon) dx \\
&= \langle -\Delta \phi, \phi - \varphi_\varepsilon \rangle - \int_\Omega g_2(\phi - \varphi_\varepsilon) dx
\end{aligned} \tag{2.87}$$

for every $0<\varepsilon<\delta$. For $\varepsilon\to 0$ this leads to

$$0\le\langle -\Delta\phi,\phi-\varphi^*\rangle-\int_\Omega g_2(\phi-\varphi^*)dx. \tag{2.88}$$

Since $\delta>0$ can be chosen arbitrarily small, the last relation holds for every $\phi\in\mathbb{K}$ via a limiting process. Applying [133, III: Lemma 1.5] once more, this implies

$$0\le\langle -\Delta\varphi^*,\phi-\varphi^*\rangle-\int_\Omega g_2(\phi-\varphi^*)dx,\ \forall\phi\in\mathbb{K}. \tag{2.89}$$

This yields the assertion, due to the uniqueness of the solution for our variational inequality problem. □

We argue similarly concerning the regularity of $\mu\in\overline{H}^1$. Indeed, first note that by Sobolev‘s embedding theorem and Hölder’s inequality, $g_3:=\frac{\varphi-\tilde\varphi}{\tau}+v\nabla\tilde\varphi-\Theta_\mu-\mu$ is an element of $L^2(\Omega)$. Furthermore, the coefficient function $m(\tilde\varphi)$ is contained in the Sobolev spaces $H^2(\Omega)$ and $W^{1,6}(\Omega)$ (cf. [133, II, Lemma A.3]). Once more we apply [144, Theorem 2.3.5] and [144, Theorem 2.3.1] to conclude that the problem

$$m(\tilde\varphi)\Delta\mu^*+\nabla(m(\tilde\varphi))\nabla\mu^*-\mu^*=g_3 \text{ a.e. in }\Omega,\ \partial_n\varphi_{|\partial\Omega}=0\text{ on }\partial\Omega, \tag{2.90}$$

has a strong solution $\mu^*\in\overline{H}^2_{\partial_n}(\Omega)$ which coincides with μ and it holds that

$$\|\mu\|_{H^2}\le C(\|\mu\|+\|g_3\|)\le C(\|\mu\|+\|\varphi\|+\|\tilde\varphi\|+\|v\|_{H^1}\|\tilde\varphi\|_{H^2}+\left\|\Theta_\mu\right\|), \tag{2.91}$$

where $C>0$ depends only on N,Ω,b_1,b_2,τ.

Finally, we show the desired regularity of v. For an arbitrary test function $\psi\in C^\infty_{0,\sigma}(\Omega;\mathbb{R}^N)$ it holds by equation (2.48c) that

$$\begin{aligned}(2\eta(\tilde\varphi)\varepsilon(v),\nabla\psi)&=\left(\operatorname{div}(v\otimes\nu)+\frac{1}{\tau}(f_0v-f_{-1}\tilde v)-\mu\nabla\tilde\varphi-\Theta_v,\psi\right)\\&=:(f,\psi)\end{aligned}$$

with $||f||\le C(z)$ for a constant $C(z)>0$ depending only on

$$z=(N,\Omega,\eta,\tau,||\nu||_{H^1},||v||_{H^1},||\varphi||_{H^2},||\tilde\varphi||_{H^2},||\mu||_{H^2},||\Theta_v||).$$

Moreover, $\operatorname{div}(v\otimes\nu)=(Dv)\nu+v\operatorname{div}\nu$. Using a modified test function $\hat\psi:=\eta(\tilde\varphi)^{-1}\psi-B[\operatorname{div}(\eta(\tilde\varphi)^{-1}\psi)]\in H^1_{0,\sigma}(\Omega;\mathbb{R}^N)$ (where B denotes the Bogovskiĭ operator introduced in [33]), we derive the following equation, cf. [2],

$$
\begin{aligned}
(\varepsilon(v),\nabla\psi) =& (\eta(\tilde{\varphi})\varepsilon(v),\nabla(\eta(\tilde{\varphi})^{-1}\psi)) - (\eta(\tilde{\varphi})\varepsilon(v),(\nabla\eta(\tilde{\varphi})^{-1})\otimes\psi) \\
=& (f,\eta(\tilde{\varphi})^{-1}\psi) - (f,B[(\nabla\eta(\tilde{\varphi})^{-1})\psi]) \\
& + (\eta(\tilde{\varphi})\varepsilon(v),\nabla B[(\nabla\eta(\tilde{\varphi})^{-1})\psi]) \qquad (2.92)\\
& - (\eta(\tilde{\varphi})\varepsilon(v),(\nabla\eta(\tilde{\varphi})^{-1})\otimes\psi) =: (\tilde{f},\psi). \qquad (2.93)
\end{aligned}
$$

In order to show $v \in H^2(\Omega;\mathbb{R}^N)$, we apply a bootstrap argument and well-known regularity results for the stationary Stokes' equation, cf. [78].

Since $v \in H^1_{0,\sigma}(\Omega;\mathbb{R}^N)$, we have that $(Dv)v$, $v\operatorname{div} v$ and, as a consequence, f and $\tilde{f}$ belong to $L^{3/2}(\Omega;\mathbb{R}^N)$. Therefore, [78, Chapter IV, Lemma 6.1] and (2.93) show that $v \in W^{2,3/2}(\Omega;\mathbb{R}^N)$ and that $||v||_{W^{2,3/2}} \le C(z)$ for a constant C depending only on z.

Next, $v \in W^{2,3/2}(\Omega;\mathbb{R}^N)$ and the continuous embedding of $W^{1,3/2}(\Omega)$ into $L^3(\Omega)$ (which we denote by $W^{1,3/2}(\Omega) \hookrightarrow L^3(\Omega)$) imply that $(Dv)v$ belongs to $L^2(\Omega;\mathbb{R}^N)$. Moreover, $W^{2,3/2}(\Omega) \hookrightarrow L^p(\Omega)$ for every $p < \infty$. Hence $v\operatorname{div} v, f, \tilde{f} \in L^{2-\varepsilon}(\Omega;\mathbb{R}^N)$ for every $\varepsilon > 0$. Applying [78, Chapter IV, Lemma 6.1] again yields $v \in W^{2,2-\varepsilon}(\Omega;\mathbb{R}^N)$ for all $\varepsilon > 0$ and $||v||_{W^{2,2-\varepsilon}} \le C(\varepsilon, z)$.

Finally, having $v \in W^{2,2-\varepsilon}(\Omega;\mathbb{R}^N)$ and since $W^{2,2-\varepsilon}(\Omega) \hookrightarrow L^\infty(\Omega)$ for ε sufficiently small, it follows that also $v\operatorname{div} v$ belongs to $L^2(\Omega;\mathbb{R}^N)$. Thus, we arrive at $v \in H^2(\Omega;\mathbb{R}^N)$ and $||v||_{H^2} \le C(z)$.

This completes the proof. □

Note that Lemma 2.2.2 ensures that the initial data (for the next time step) associated with a solution of system (2.48) for a given time step via the setting from Remark 2.2.1 is sufficiently regular such that the system (2.48) for the next time step is well-posed and solvable via Theorem 2.2.1.

2.2.2 The semi-discrete Cahn–Hilliard–Navier–Stokes system

In this section we consider the complete semi-discrete Cahn–Hilliard–Navier–Stokes system (2.37). Our goal is verify the existence of solutions for all time instances via repeated applications of the results of the previous section. For the case of the double-obstacle potential, these results can be directly transferred to the system (2.37) by using the setting of Remark 2.2.1.

However, for double-well-type potentials the application of the setting (2.49) is not straight forward. Since the density function is cut off at zero by the max-operator (cf. (2.36)), the functions

$$f_0 = \rho(\varphi_i),\ f_{-1} = \rho(\varphi_{i-1}),\ v = \rho(\varphi_{i-1})v_i - \frac{\rho_2-\rho_1}{2}m(\varphi_{i-1})\nabla\mu_i \tag{2.94}$$

may not satisfy equation (2.50) if φ_i attains arbitrary values in $\mathbb{R}$ and $\rho(\varphi_i)$ becomes zero. We overcome this difficulty by applying Theorem 2.2.1 with the following setting

$$\begin{aligned}&\tilde{v} := v_i,\ \tilde{\varphi} := \varphi_i,\ f_0 := \rho(\varphi_i),\ f_{-1} := \rho(\varphi_{i-1}),\\ &v := \overline{v}(\varphi_{i-1},\varphi_i,\mu_i,v_i),\ \Theta_v := u_{i+1},\ \Theta_\varphi := \Theta_\mu := 0,\end{aligned} \tag{2.95}$$

where $\overline{v} : H^1_{0,\sigma}(\Omega;\mathbb{R}^N)\times\overline{H}^2(\Omega)^3 \to H^1(\Omega;\mathbb{R}^N)$ is given by

$$\overline{v}(\tilde{\varphi},\varphi,v,\mu) := \begin{cases} \rho(\tilde{\varphi})v - \frac{\rho_2-\rho_1}{2}m(\tilde{\varphi})\nabla\mu & \text{if } \rho(\varphi),\rho(\tilde{\varphi})>0 \text{ a.e. in } \Omega,\\ G\left(\frac{\rho(\varphi)-\rho(\tilde{\varphi})}{\tau}\right) & \text{else.}\end{cases} \tag{2.96}$$

Here $G : L^2(\Omega)\to H^1(\Omega;\mathbb{R}^N), \delta\longmapsto\zeta$ denotes an arbitrary solution operator of the equation

$$-\mathrm{div}\zeta = \delta \text{ a.e. on } \Omega. \tag{2.97}$$

We point out that a potential realization of G can be obtained by defining $\zeta := \nabla\xi \in H^1(\Omega,\mathbb{R}^N)$, where $\xi\in H^2(\Omega)\cap H^1_0(\Omega)$ solves the system

$$-\Delta\xi = \delta, \text{ a.e. on } \Omega \tag{2.98}$$

$$\xi = 0 \text{ a.e. on } \partial\Omega. \tag{2.99}$$

The double-obstacle potential

Utilizing the setting (2.95), we show the existence of solutions to a slightly modified Cahn-Hilliard-Navier-Stokes system. More precisely, we study the system

(2.37a),(2.37b),(2.100), where the Navier-Stokes equation (2.37c) is replaced by

$$\begin{aligned}\left\langle\frac{\rho(\varphi_i)v_{i+1}-\rho(\varphi_{i-1})v_i}{\tau},\psi\right\rangle_{H^{-1}_{0,\sigma},H^1_{0,\sigma}}&+(2\eta(\varphi_i)\varepsilon(v_{i+1}),\varepsilon(\psi))\\ -\langle v_{i+1}\otimes\overline{v}(\varphi_{i-1},\varphi_i,\mu_i,v_i),\nabla\psi\rangle_{H^{-1}_{0,\sigma},H^1_{0,\sigma}}&-\langle\mu_{i+1}\nabla\varphi_i,\psi\rangle_{H^{-1}_{0,\sigma},H^1_{0,\sigma}}\\ =\langle u_{i+1},\psi\rangle_{H^{-1}_{0,\sigma},H^1_{0,\sigma}},&\ \forall\psi\in H^1_{0,\sigma}(\Omega;\mathbb{R}^N)\end{aligned}\tag{2.100}$$

for each time step.

Nevertheless, we emphasize that for the double-obstacle potential the modified system (2.37a),(2.37b),(2.100) coincides with the semi-discrete Cahn-Hilliard-Navier-Stokes system (2.37). As φ_i is contained in the interval $[\psi_1,\psi_2]$ for every time instance i, it holds that

$$\rho(\varphi_{i-1})\geq\rho(\psi_1)=\rho_1>0\wedge\rho(\varphi_i)>0\text{ a.e. on }\Omega.\tag{2.101}$$

Hence, the definition of $\overline{v}$ in (2.96) ensures that

$$\overline{v}(\varphi_{i-1},\varphi_i,\mu_i,v_i)=\rho(\varphi_{i-1})v_i-\frac{\rho_2-\rho_1}{2}m(\varphi_{i-1})\nabla\mu_i.\tag{2.102}$$

As a consequence, the solutions obtained in the subsequent theorem satisfy the original Cahn-Hilliard-Navier-Stokes system (2.37).

Theorem 2.2.2 (Existence of solution to the modified system)**.** *Suppose that $u\in L^2(\Omega;\mathbb{R}^N)^{M-1}$ and $\overline{v}:H^1_{0,\sigma}(\Omega;\mathbb{R}^N)\times\overline{H}^1(\Omega)^3\to H^1(\Omega;\mathbb{R}^N)$ are defined by (2.96).*

Then there exists a point

$$(\varphi,\mu,v)\in\overline{H}^2_{\partial_n}(\Omega)^M\times\overline{H}^2_{\partial_n}(\Omega)^M\times H^1_{0,\sigma}(\Omega;\mathbb{R}^N)^{M-1},\tag{2.103}$$

which solves the semi-discrete system (2.37a),(2.37b),(2.100).

Moreover, every solution of the system (2.37a),(2.37b),(2.100) is contained in the product space $\overline{H}^2_{\partial_n}(\Omega)^M\times\overline{H}^2_{\partial_n}(\Omega)^M\times H^1_{0,\sigma}(\Omega;\mathbb{R}^N)^{M-1}$.

Proof. Standard arguments guarantee the existence of $(\varphi_0,\mu_0)\in\overline{H}^1(\Omega)\times\overline{H}^1(\Omega)$ such that (2.37a)-(2.37b) is satisfied for $i=-1$. Lemma 2.2.2 yields $(\varphi_0,\mu_0)\in\overline{H}^2_{\partial_n}(\Omega)\times\overline{H}^2_{\partial_n}(\Omega)$.

Let $(\varphi_{i-1},\varphi_i,\mu_i,v_i)\in\overline{H}^2_{\partial_n}(\Omega)\times\overline{H}^2_{\partial_n}(\Omega)\times\overline{H}^2_{\partial_n}(\Omega)\times H^1_{0,\sigma}(\Omega;\mathbb{R}^N)$ be given for $i\geq 0$. Note that $\overline{v}(\varphi_{i-1},\varphi_i,\mu_i,v_i)$, as defined in (2.96), is contained in $H^1(\Omega)$. If condition (2.101) holds true, then Assumption 2.1.1 (*III*) and (2.37a) imply

$$\begin{aligned}\operatorname{div}\overline{v}(\varphi_{i-1},\varphi_i,\mu_i,v_i)&=\frac{\rho_2-\rho_1}{2}(\nabla\varphi_{i-1}v_i-\operatorname{div}(m(\varphi_{i-1})\nabla\mu_i))&(2.104)\\ &=-\frac{\rho_2-\rho_1}{2}(\frac{\varphi_i-\varphi_{i-1}}{\tau})&(2.105)\\ &=-\frac{\rho(\varphi_i)-\rho(\varphi_{i-1})}{\tau}.&(2.106)\end{aligned}$$

Hence, if (φ_i, μ_i, v_i) satisfies (2.37a), then Assumption (2.50) is always satisfied by the definition of $\overline{v}$ in the sense that

$$\frac{\rho(\varphi_i) - \rho(\varphi_{i-1})}{\tau} + \operatorname{div}\overline{v}(\varphi_{i-1}, \varphi_i, \mu_i, v_i) = 0 \text{ a.e. on } \Omega. \tag{2.107}$$

Therefore we can apply Theorem 2.2.1 with the setting (2.95) to guarantee the existence of $(\varphi_{i+1}, \mu_{i+1}, v_{i+1}) \in \overline{H}^1(\Omega) \times \overline{H}^1(\Omega) \times H^1_{0,\sigma}(\Omega;\mathbb{R}^N)$ such that the system (2.37a),(2.37b),(2.100) is satisfied.

Now Lemma 2.2.2 yields $(\varphi_{i+1}, \mu_{i+1}, v_{i+1}) \in \overline{H}^2_{\partial_n}(\Omega) \times \overline{H}^2_{\partial_n}(\Omega) \times H^1_{0,\sigma}(\Omega;\mathbb{R}^N)$. In the case of the double-obstacle potential it additionally follows that $\varphi_1 \in \mathbb{K}$.

Repeated applications of Theorem 2.2.1 and Lemma 2.2.2 for each time step $i = 0,..,M-2$ prove the assertion. □

Using Lemma 2.2.1, we can also establish a global energy estimate for the modified system (2.37a),(2.37b),(2.100) for all time steps. This guarantees that the solutions of the system remain bounded in their respective H^2-spaces.

Lemma 2.2.4 (Boundedness of the state)**.** *Let the assumptions from Theorem 2.2.2 be fulfilled and*

$$(\varphi, \mu, v) \in \overline{H}^2_{\partial_n}(\Omega)^M \times \overline{H}^2_{\partial_n}(\Omega)^M \times H^1_{0,\sigma}(\Omega;\mathbb{R}^N)^{M-1} \tag{2.108}$$

be a solution of the system (2.37a),(2.37b),(2.100).

Then there exists a positive constant $C = C(N, \Omega, b_1, b_2, \tau, \kappa, v_a, \varphi_a, u) > 0$ *such that*

$$\|v\|^2_{(H^2)^M} + \|\mu\|^2_{(H^2)^M} + \|\varphi\|^2_{(H^2)^{M+1}} \leq C. \tag{2.109}$$

Furthermore, the operator $L^2(\Omega,\mathbb{R}^N)^{M-1} \to \mathbb{R}, u \longmapsto C(N, \Omega, b_1, b_2, \tau, \kappa, v_a, \varphi_a, u)$ *is bounded.*

Proof. We recall that the semi-discrete total energy functional $E : \overline{H}^1_{0,\sigma}(\Omega) \times \overline{H}^1(\Omega) \times \overline{H}^1(\Omega) \to \mathbb{R}$ was defined as

$$E(v, \varphi, \phi) := \int_\Omega \frac{\rho(\phi)\,|v|^2}{2} dx + \int_\Omega \frac{|\nabla\varphi|^2}{2} dx + \Psi(\varphi). \tag{2.110}$$

Let $j \in \{1,..,M-2\}$ be arbitrarily fixed. Then by repeatedly applying Lemma

2.2.1 with the setting (2.95) for $i = j, j-1, .., 0$, we can conclude that

$$
\begin{aligned}
& E(v_{j+1}, \varphi_{j+1}, \varphi_j) + \tau \int_\Omega 2\eta(\varphi_j) \left|\varepsilon(v_{j+1})\right|^2 dx + \tau \int_\Omega m(\varphi_j) \left|\nabla \mu_{j+1}\right|^2 dx \\
& \leq E(v_j, \varphi_j, \varphi_{j-1}) + \left(u_{j+1}, v_{j+1}\right) \\
& \leq E(v_{j-1}, \varphi_{j-1}, \varphi_{j-2}) + \left(u_j, v_j\right) + \left(u_{j+1}, v_{j+1}\right) \\
& \vdots \\
& \leq E(v_0, \varphi_0, \varphi_{-1}) + \sum_{i=1}^{j+1} (u_i, v_i)\,.
\end{aligned}
$$

By Assumptions 2.1.1 and 2.1.2 this yields

$$
\begin{aligned}
& \int_\Omega \frac{\left|\nabla \varphi_{j+1}\right|^2}{2} dx + \Psi(\varphi_{j+1}) + 2\tau b_1 \int_\Omega \left|\varepsilon(v_{j+1})\right|^2 dx + \tau b_1 \int_\Omega \left|\nabla \mu_{j+1}\right|^2 dx \\
& \leq E(v_0, \varphi_0, \varphi_{-1}) + \sum_{i=1}^{M-1} \|u_i\| \, \|v_i\| \leq C_1 + C_2 \|u\|_{(L^2)^{M-1}} \|v\|_{(H^1)^M}\,, \qquad (2.111)
\end{aligned}
$$

where C_1 depends only on the initial data $(N, \Omega, B_l, B_u, v_a, \varphi_a)$. Due to Korn's inequality and Poincaré's inequality, this ensures

$$
\left\|v_{j+1}\right\|_{H^1}^2 + \left\|\mu_{j+1}\right\|_{H^1}^2 + \left\|\varphi_{j+1}\right\|_{H^1}^2 \leq C_1 + C_2 \|u\|_{(L^2)^{M-1}} \|v\|_{(H^1)^M}\,.
$$

Since $j \in \{1, .., M-1\}$ is arbitrarily chosen, we infer

$$
\|v\|_{(H^1)^M}^2 + \|\mu\|_{(H^1)^M}^2 + \|\varphi\|_{(H^1)^{M+1}}^2 \leq C_1 + C_2 \left(\|u\|_{(L^2)^{M-1}} \|v\|_{(H^1)^M} \right). \qquad (2.112)
$$

Hence (φ, μ, v) is bounded in $\overline{H}^1(\Omega)^M \times \overline{H}^1(\Omega)^M \times H^1_{0,\sigma}(\Omega; \mathbb{R}^N)^{M-1}$. The boundedness in the respective H^2-spaces then follows directly by applying Lemma 2.2.2 for each time step. □

Double-well type potentials

In the following, we address the case of free energies of double-well type, cf. Assumption 2.1.2.2. As discussed above, the modified system (2.37a),(2.37b),(2.100) differs from the original Cahn–Hilliard–Navier–Stokes system (2.37) if the order parameter is far below the interval $[\psi_1, \psi_2]$. However, in the subsequent theorem we assure that the order parameter remains in a close neighborhood of $[\psi_1, \psi_2]$ if the double-well type potential is close to the double-obstacle potential in a certain sense specified in condition (II).

Theorem 2.2.3. *Let $u \in L^2(\Omega;\mathbb{R}^N)^{M-1}$ be given and $\left\{\Psi_0^{(k)}\right\}_{k\in\mathbb{N}}$ a sequence of functions which satisfies the following two conditions:*

(I) The functional $\Psi_0^{(k)}$ fulfills Assumption 2.1.2 for every $k \in \mathbb{N}$.

(II) If $\left\{\hat{\varphi}^{(k)}\right\}_{k\in\mathbb{N}}$ is a sequence in $\overline{H}^1(\Omega)$ such that there exists $C > 0$ with $\Psi_0^{(k)}\left(\hat{\varphi}^{(k)}\right) \leq C$ for every $k \in \mathbb{N}$, then

$$\left\|\max(-\hat{\varphi}^{(k)} + \psi_1, 0)\right\|_{L^1} \to 0, \text{ as } k \to \infty.$$

Furthermore, let $\left\{(\varphi^{(k)}, \mu^{(k)}, \nu^{(k)})\right\}_{k\in\mathbb{N}}$ be a sequence of solutions to the systems (2.37a),(2.37b),(2.100) with $\Psi_0 = \Psi_0^{(k)}$. Then

$$\left\|\max(-\varphi^{(k)} + \psi_1, 0)\right\|_{L^\infty} \to 0, \text{ as } k \to \infty.$$

Proof. Employing Lemma 2.2.4, and in particular inequality (2.111), we see that for every $i \in \{-1, .., M-1\}$ and $k \in \mathbb{N}$ it holds that $\Psi^{(k)}(\varphi_i^{(k)}) \leq C_1$. Hence we conclude

$$\Psi_0^{(k)}\left(\varphi_i^{(k)}\right) \leq C_1 + \frac{\kappa}{2}\left\|\varphi_i^{(k)}\right\|_{L^2}^2 \leq C_2.$$

By assumption (II), this yields

$$\left\|\max(-\varphi_i^{(k)} + \psi_1, 0)\right\|_{L^1} \to 0 \text{ for } k \to \infty. \tag{2.113}$$

Next, we use the technique of [114, Proposition 2.4] and [114, Remark 2.5] to derive that $\left\|\max(-\varphi_i^{(k)} + \psi_1, 0)\right\|_{L^\infty} \to 0$ for $k \to \infty$. We stay brief here and refer to [114] for details on the technique.

By Lemma 2.2.4 the sequence $\left\{\varphi^{(k)}\right\}_{k\in\mathbb{N}}$ is bounded in $\overline{H}^2(\Omega)$ and, due to Sobolev's embedding theorem, in $W^{1,6}(\Omega)$ and $C^{0,\beta}(\overline{\Omega})$, $\beta \leq \frac{1}{2}$. Thus, there exists a constant C_β such that for every $k \in \mathbb{N}$ we have $\left\|\varphi^{(k)}\right\|_{C^{0,\beta}} \leq C_\beta$.

For fixed $k \in \mathbb{N}$ assume that $\left\|\max(-\varphi_i^{(k)} + \psi_1, 0)\right\|_{L^\infty} > 0$ and define the set $\mathbb{G} := \left\{\omega \in \overline{\Omega} : \varphi_i^{(k)}(\omega) \leq \psi_1 < 0\right\}$. Then let $\omega_{max} \in \mathbb{G}$ satisfy

$$-\varphi_i^{(k)}(\omega_{max}) + \psi_1 = \left\|-\varphi_i^{(k)} + \psi_1\right\|_{L^\infty(\mathbb{G})} = \left\|\max(-\varphi_i^{(k)} + \psi_1, 0)\right\|_{L^\infty(\Omega)}.$$

Due to the Hölder continuity of $\varphi_i^{(k)}$, for every $x \in \Omega$ which satisfies $|x - \omega_{max}|_{\mathbb{R}^N} \leq \left(\frac{-\varphi_i^{(k)}(\omega_{max}) + \psi_1}{2C_\beta} \right)^{\frac{1}{\beta}}$ it holds that

$$\begin{aligned} -\varphi_i^{(k)}(x) + \psi_1 &\geq -\varphi_i^{(k)}(\omega_{max}) + \psi_1 - \left\| \varphi_i^{(k)} \right\|_{C^{(0,\beta)}(\Omega)} |\omega_{max} - x|_{\mathbb{R}^N}^\beta \\ &\geq \frac{-\varphi_i^{(k)}(\omega_{max}) + \psi_1}{2} > 0. \end{aligned}$$

As Ω satisfies the cone condition, there exists a finite cone $K_r(\omega_{max}) := K(\omega_{max}) \cap B(\omega_{max}, r)$ of radius r and with vertex ω_{max} such that $K_r(\omega_{max}) \subset \Omega$. Hence the cone $K_R(\omega_{max})$ with $R := \min \left(r, \left(\frac{-\varphi_i^{(k)}(\omega_{max}) + \psi_1}{2C_\beta} \right)^{\frac{1}{\beta}} \right)$ is contained in $\mathbb{G}$. Consequently, we find

$$\begin{aligned} \left\| \max(-\varphi_i^{(k)} + \psi_1, 0) \right\|_{L^1(\Omega)} &\geq \int_{K_R(\omega_{max})} -\varphi_i^{(k)} + \psi_1 dx \\ &\geq \int_{K_R(\omega_{max})} \frac{\left(-\varphi_i^{(k)}(\omega_{max}) + \psi_1 \right)}{2} dx \\ &\geq \frac{|K_R(0)|}{2} \left\| \max(-\varphi_i^{(k)} + \psi_1, 0) \right\|_{L^\infty(\Omega)}. \end{aligned}$$

In combination with (2.113) this proves the assertion. □

Let us define $\varphi^- \in \mathbb{R}$ as

$$\varphi^- := \inf\{\varphi \in \mathbb{R} : \rho(\varphi) > 0\} < \psi_1. \tag{2.114}$$

As in Theorem 2.2.3, we consider an arbitrary force $u \in L^2(\Omega; \mathbb{R}^N)^{M-1}$ and a sequence $\left\{ \Psi_0^{(k)} \right\}_{k \in \mathbb{N}}$ of double-well type potentials which satisfy condition (II). Then there exists $k^* \in \mathbb{N}$ such that for every $k \geq k^*$ the solutions $(\varphi^{(k)}, \mu^{(k)}, v^{(k)})$ to the corresponding system (2.37a),(2.37b),(2.100) with $\Psi_0 = \Psi_0^{(k)}$ satisfy

$$\varphi_i^{(k)} > \varphi^-, \ \forall i = -1, .., M-1. \tag{2.115}$$

Thus the inequalities (2.101) hold true for every $i = -1, .., M-1$ and $k \geq k^*$ and equation (2.100) coincides with the discretized Navier–Stokes equation (2.37c). This gives rise to the subsequent theorem.

Theorem 2.2.4 (Existence of feasible points). *Let $u \in L^2(\Omega; \mathbb{R}^N)^{M-1}$ be given and let $\left\{ \Psi_0^{(k)} \right\}_{k \in \mathbb{N}}$ be a sequence satisfying the assumptions of Theorem 2.2.3.*

Then there exists a $k^* \in \mathbb{N}$ such that the system (2.37) *with $\Psi_0 = \Psi_0^{(k)}$ admits a solution*

$$(\varphi, \mu, v) \in \overline{H}^2_{\partial_n}(\Omega)^M \times \overline{H}^2_{\partial_n}(\Omega)^M \times H^1_{0,\sigma}(\Omega;\mathbb{R}^N)^{M-1} \tag{2.116}$$

for every $k \geq k^*$. Moreover, the results of Lemma 2.2.4 hold true.

In summary, we have shown that the semi-discrete Cahn–Hilliard–Navier–Stokes system (2.37) possesses a solution for the double-obstacle potential and for certain double-well type potentials which are close to the double-obstacle potential. In the following sections we focus our research on these two cases.

Returning to our initial observations, we note that the existence of solutions to the time-continuous Cahn–Hilliard–Navier–Stokes system can now be established via a limiting process with respect to the total number of time instances $M \to \infty$ and the time step size $\tau := \frac{T}{M} \to 0$. For this purpose, one considers certain step functions f^M_{step} with respect to the time t which are equal to the time discrete solutions on each interval $t \in [(i-1)\tau, i\tau)$ for $i = 1, .., M-1$, i.e.

$$f^M_{step}(t) = f_i, \; f \in \{v, \varphi, \mu\}.$$

With the help of the energy estimate (2.51) these functions can be bounded in the spaces $v^M_{step} \in L^2(0,T,H^1(\Omega;\mathbb{R}^n))$, $\varphi^M_{step} \in L^\infty(0,T,H^1(\Omega))$, and $\mu^M_{step} \in L^2(0,T,H^1(\Omega))$, respectively. This guarantees the existence of a weakly convergent subsequence whose limit point can be shown to fulfill the system (2.27).

However, since these arguments cannot be directly transferred to the adjoint system associated with the optimal control problem and the study of the time-continuous Cahn–Hilliard–Navier–Stokes system lies beyond the scope of this thesis, we restrict our investigations on the semi-discrete system. For more details on the existence of solutions for the fully continuous system we refer to, e.g., [4], where this approach has been successfully applied to the case where the free energy density is defined through the logarithmic potential given in (2.9).

Chapter 3

The optimal control problem

3.1 Problem formulation

In this chapter, we present the optimal control problem associated with the semi-discrete Cahn–Hilliard–Navier–Stokes system, the central object of our research. We proceed with an existence proof which verifies the existence of global solutions to the optimal control problem, followed by a short discussion of the associated stationarity concepts.

In order to formulate the optimal control problem we consider an arbitrary objective function $\mathscr{J} : \mathscr{X} \to \mathbb{R}$ defined on the product space

$$\mathscr{X} := \overline{H}^1(\Omega)^M \times \overline{H}^1(\Omega)^M \times H^1_{0,\sigma}(\Omega;\mathbb{R}^n)^{M-1} \times L^2(\Omega;\mathbb{R}^n)^{M-1}. \tag{3.1}$$

Definition 3.1.1. *The optimal control problem is given by*

$$\begin{aligned}&\min \mathscr{J}(\varphi,\mu,v,u) \text{ over } (\varphi,\mu,v,u) \in \mathscr{X}\\ &\text{s.t. } u \in U_{ad},\ (\varphi,\mu,v) \in S_\Psi(u),\end{aligned} \tag{P_Ψ}$$

where S_Ψ is the solution operator of the semi-discrete Cahn–Hilliard–Navier–Stokes system, cf. (2.38).

Note that we include the case of additional constraints on the control u by adding the constraint set

$$U_{ad} \subset L^2(\Omega;\mathbb{R}^n)^{M-1}. \tag{3.2}$$

Based on our preceding observations, we can already guarantee that the feasible set of problem (P_Ψ) is non-empty if $U_{ad} \neq \emptyset$.

Due to the generality of the problem formulation, it is relatively hard to derive any meaningful results for the optimal control problem (P_Ψ) without imposing further assumptions on the data. That is why we make the following assumptions for the constraint set and the objective functional.

Assumption 3.1.1. *We suppose that*

(I) *U_{ad} is non-empty, closed and convex;*

(II) *$\mathscr{J}$ is convex and weakly lower-semi-continuous;*

(III) *either U_{ad} is bounded or $\mathscr{J}$ is partially coercive, i.e. for every sequence $\left\{(\varphi^{(k)},\mu^{(k)},v^{(k)},u^{(k)})\right\}_{k\in\mathbb{N}}$ with $\lim_{k\to\infty}\left\|u^{(k)}\right\| = \infty$ it holds that*

$$\lim_{k\to\infty} \mathscr{J}(\varphi^{(k)},\mu^{(k)},v^{(k)},u^{(k)}) = \infty.$$

We point out that these are classical assumptions in the literature on optimization theory, which ensure, e.g., that the optimal control problem is well-posed. For the derivation of necessary first-order optimality conditions later on we additionally assume that $\mathscr{J}$ is Fréchet differentiable for the ease of exposition.

However, we emphasize that many important objective functionals, which are used in practical applications, satisfy these assumptions. In particular, we mention that objective functionals of tracking type such as

$$\mathscr{J}(\varphi, \mu, v, u) := \frac{1}{2} \sum_{i=1}^{M-1} \left\| \varphi_i - \varphi_{d,i} \right\|^2 + \frac{\xi}{2} \|u\|^2_{(L^2)^{(M-1)}}, \tag{3.3}$$

or

$$\mathscr{J}(\varphi, \mu, v, u) := \frac{1}{2} \|\varphi_{M-1} - \varphi_d\|^2 + \frac{\xi}{2} \|u\|^2_{(L^2)^{(M-1)}}, \tag{3.4}$$

where the distance to a desired state $\varphi_d \in L^2(\Omega)$ is minimized while penalizing the control cost via the parameter $\xi > 0$, are convex, weakly lower-semi-continuous and partially coercive.

The boundary control problem

For some applications, a boundary control might be easier to realize than the distributed control introduced in Definition 3.1.1. Here, the homogeneous boundary of the velocity field is omitted in favor of the boundary condition

$$v_{i+1|\partial\Omega} = u_{i+1}. \tag{3.5}$$

In this case, the control u_{i+1} is an element of the space $H_{tr} := Tr(H^1_\sigma(\Omega;\mathbb{R}^n))$, where Tr denotes the zero-order trace operator, cf., e.g., [7]. Due to the embedding properties of Sobolev spaces, H_{tr} is contained in $H^{\frac{1}{2}}(\partial\Omega;\mathbb{R}^n)$. Moreover, it is a Hilbert space and the trace operator regarded from $H^1_\sigma(\Omega;\mathbb{R}^n)$ into H_{tr} is a linear, bounded and surjective mapping between Hilbert spaces. Hence, there exists a right inverse operator $B_{tr} : H_{tr} \to H^1_\sigma(\Omega;\mathbb{R}^n)$ such that $Tr \circ B_{tr}$ equals the identity operator on H_{tr}, cf. [16, 96].

The operator can be employed to reduce the inhomogeneous Navier–Stokes system to the problem with homogeneous Dirichlet boundary conditions, which is used in [118], to derive the existence of solutions to the Cahn-Hilliard-Navier-Stokes system via similar arguments as in Chapter 2 (namely Brouwer's fix point theorem and monotone operator theory). In the aforementioned article, a boundary-control equivalent of the problem (P_Ψ) is studied with a tracking-type functional for matched densities. Furthermore, the constraint set U_{ad} is assumed to be a closed, linear subspace of H_{tr} and an additional compatibility condition on the given data is imposed.

Although we focus on the optimal control problem subject to a distributed control in this thesis, we point out that most of our arguments can be transferred to the case of boundary controls due to the linearity of the trace operator. In combination with a careful embedding analysis with respect to the involved trace spaces as sketched above, this paves the road to a stationarity system of C-stationary type for the respective boundary control problem, see also [118].

3.2 Existence of globally optimal points

This section is devoted to the well-posedness of the optimal control problem (P_Ψ). More precisely, we confirm the existence of globally optimal points for (P_Ψ). For this purpose, we assume that the given data satisfies the assumptions made in the previous sections, in particular the Assumptions 2.1.1 and 3.1.1.

The proof of the subsequent theorem follows the guideline presented in Section 1.3 and heavily relies on various imbedding properties of Sobolev spaces introduced in Section 1.2.

Theorem 3.2.1 (Existence of global solutions)**.** *The optimization problem (P_Ψ) admits a global solution.*

Proof. By Theorem 2.2.2 the feasible set of the problem (P_Ψ) is non-empty and contained in $\overline{H}^2_{\partial_n}(\Omega)^M \times \overline{H}^2_{\partial_n}(\Omega)^M \times H^1_{0,\sigma}(\Omega;\mathbb{R}^N)^{M-1} \times U_{ad}$.

Let $\left\{(\varphi^{(k)},\mu^{(k)},v^{(k)},u^{(k)})\right\}_{k\in\mathbb{N}}$ be an infimizing sequence of $\mathscr{J}$ in $\overline{H}^2_{\partial_n}(\Omega)^M \times \overline{H}^2_{\partial_n}(\Omega)^M \times H^1_{0,\sigma}(\Omega;\mathbb{R}^N)^{M-1} \times U_{ad}$ with $(\varphi^{(k)},\mu^{(k)},v^{(k)}) \in S_\Psi(u^{(k)})$ such that

$$\lim_{k\to\infty} \mathscr{J}(\varphi^{(k)},\mu^{(k)},v^{(k)},u^{(k)}) = \inf_{u\in U_{ad},(\varphi,\mu,v)\in S_\Psi(u)} \mathscr{J}(\varphi,\mu,v,u). \tag{3.6}$$

Note that the infimum on the right-hand side may be $-\infty$. The sequence $\left\{u^{(k)}\right\}_{k\in\mathbb{N}}$ is bounded in the reflexive Banach space $L^2(\Omega;\mathbb{R}^N)^{M-1}$. This follows either directly from the boundedness of the set U_{ad} or from the partial coercivity of $\mathscr{J}$.

Then by Lemma 2.2.4 the sequence $(\varphi^{(k)},\mu^{(k)},v^{(k)})$ is bounded in $\overline{H}^2_{\partial_n}(\Omega)^M \times \overline{H}^2_{\partial_n}(\Omega)^M \times H^1_{0,\sigma}(\Omega;\mathbb{R}^N)^{M-1}$. Setting

$$\left\{w^{(k)}\right\}_{k\in\mathbb{N}} := \left\{(\varphi^{(k)},\mu^{(k)},v^{(k)},u^{(k)})\right\}_{k\in\mathbb{N}}, \tag{3.7}$$

there exists a weakly convergent subsequence $\left\{w^{(k_l)}\right\}_{l\in\mathbb{N}}$ with limit point

$$w^* := (\varphi^*,\mu^*,v^*,u^*) \in \overline{H}^2_{\partial_n}(\Omega)^M \times \overline{H}^2_{\partial_n}(\Omega)^M \times H^1_{0,\sigma}(\Omega;\mathbb{R}^N)^{M-1}. \tag{3.8}$$

Using the weak lower-semicontinuity of $\mathscr{J}$, this implies

$$-\infty < \mathscr{J}(w^*) \le \liminf_{l\to\infty} \mathscr{J}(w^{(k_l)}) = \inf_{u\in U_{ad},(\varphi,\mu,v)\in S_\Psi(u)} \mathscr{J}(\varphi,\mu,v,u), \tag{3.9}$$

where the last equality holds due to (3.6). Since U_{ad} is weakly closed, u^* belongs to U_{ad}.

It remains to show that $(\varphi^*,\mu^*,v^*)\in S_\Psi(u^*)$. Subsequently, we slightly abuse the notation by writing l instead of k_l. We start by considering the limit of $\left\langle v_{i+1}^{(l)}\otimes\frac{\rho_2-\rho_1}{2}m(\varphi_{i-1}^{(l)})\nabla\mu_i^{(l)},\nabla\psi\right\rangle$ for arbitrary $0\le i\le M-2$ and $\psi\in H^1(\Omega;\mathbb{R}^N)$. Using the triangle and Hölder's inequality we derive

$$
\begin{aligned}
&\left\|m(\varphi_{i-1}^{(l)})\nabla\mu_i^{(l)}\cdot\nabla\psi-m(\varphi_{i-1}^*)\nabla\mu_i^*\cdot\nabla\psi\right\|_{L^{4/3}}\\
\le&\left\|m(\varphi_{i-1}^{(l)})(\nabla\mu_i^{(l)}-\nabla\mu_i^*)\cdot\nabla\psi\right\|_{L^{4/3}}\\
&+\left\|(m(\varphi_{i-1}^{(l)})-m(\varphi_{i-1}^*))\nabla\mu_i^*\cdot\nabla\psi\right\|_{L^{4/3}}\\
\le&\left\|m(\varphi_{i-1}^{(l)})\right\|_{L^\infty}\left\|\nabla\mu_i^{(l)}-\nabla\mu_i^*\right\|_{L^4}\|\nabla\psi\|_{L^2}\\
&+\left\|m(\varphi_{i-1}^{(l)})-m(\varphi_{i-1}^*)\right\|_{L^\infty}\|\nabla\mu_i^*\|_{L^4}\|\nabla\psi\|_{L^2}.
\end{aligned}
$$

Since $\nabla\mu_i^{(l)}$ converges weakly to $\nabla\mu_i^*$ in $H^1(\Omega)$ and $H^1(\Omega)$ is compactly imbedded into $L^4(\Omega)$, $\left\|\nabla\mu_i^{(l)}-\nabla\mu_i^*\right\|_{L^4}$ tends to zero for $l\to\infty$.

Due to the compact imbedding of $H^2(\Omega)$ into $W^{1,4}(\Omega)$, we have $\varphi_{i-1}^{(l)}\to\varphi_{i-1}^*$ strongly in $W^{1,4}(\Omega)$. By Assumption 2.1.1, m is Lipschitz continuous. Since $W^{1,4}(\Omega)$ can be imbedded into $L^\infty(\Omega)$, we infer $\left\|m(\varphi_{i-1}^{(l)})-m(\varphi_{i-1}^*)\right\|_{L^\infty}\to 0$.

Consequently, it holds that

$$
\frac{\rho_2-\rho_1}{2}m(\varphi_{i-1}^{(l)})\nabla\mu_i^{(l)}\cdot\nabla\psi\longrightarrow_{L^{4/3}(\Omega)}\frac{\rho_2-\rho_1}{2}m(\varphi_{i-1}^*)\nabla\mu_i^*\cdot\nabla\psi. \tag{3.10}
$$

By Sobolev's Imbedding Theorem 1.2.1 and the weak continuity of the imbedding operator, $v_{i+1}^{(l)}$ converges weakly in $L^4(\Omega)$ to v_{i+1}^*. Hence,

$$
\begin{aligned}
&\lim_{l\to\infty}\left\langle v_{i+1}^{(l)}\otimes\frac{\rho_2-\rho_1}{2}m(\varphi_{i-1}^{(l)})\nabla\mu_i^{(l)},\nabla\psi\right\rangle\\
&\quad=\left\langle v_{i+1}^*\otimes\frac{\rho_2-\rho_1}{2}m(\varphi_{i-1}^*)\nabla\mu_i^*,\nabla\psi\right\rangle
\end{aligned}\tag{3.11}
$$

One proceeds analogously for the remaining terms in the system (2.37a)-(2.37c) which do not depend on the subdifferential of Ψ_0.

In this way we also show that $\Delta\varphi_{i+1}^{(l)}+\mu_{i+1}^{(l)}+\kappa\varphi_i^{(l)}$ converges strongly in $\overline{H}^{-1}(\Omega)$ to $\Delta\varphi_{i+1}^*+\mu_{i+1}^*+\kappa\varphi_i^*$ for every $i=-1,..,M-2$, where the Laplace-operator is understood in the weak form. Furthermore, $\varphi_{i+1}^{(l)}\to\varphi_{i+1}^*$ in $\overline{H}^1(\Omega)$, and for every $l\in\mathbb{N}$ it holds that $\Delta\varphi_{i+1}^{(l)}+\mu_{i+1}^{(l)}+\kappa\varphi_i^{(l)}\in\partial\Psi_0(\varphi_{i+1}^{(l)})$.

Due to the maximal monotonicity of $\partial\Psi_0$, this implies

$$\Delta\varphi_{i+1}^* + \mu_{i+1}^* + \kappa\varphi_i^* \in \partial\Psi_0(\varphi_{i+1}^*), \tag{3.12}$$

for every $i = -1, .., M-2$. In summary, we have shown $(\varphi^*, \mu^*, v^*) \in S_\Psi(u^*)$. As a consequence, the limit point $(\varphi^*, \mu^*, v^*, u^*)$ is contained in the feasible set of the problem (P_Ψ). In combination with the inequality (3.9), this ensures that $(\varphi^*, \mu^*, v^*, u^*)$ solves the optimal control problem. $\square$

Note that we only employed the maximal monotonicity of the subdifferential of Ψ_0. Thus, Theorem 3.2.1 guarantees the existence of solutions for the double-obstacle potential as well as the double-well type potentials under consideration.

3.3 Optimality conditions

After securing the existence of solutions to the optimal control problem (P_Ψ) it is our goal to derive meaningful optimality conditions for the problem. This is not only to provide a more precise characterization of globally and/or locally optimal points, but also facilitates the development of efficient numerical solution methods to approximate these solutions.

However, we recall that in the presence of the double-obstacle potential the constraint system (2.37) of the optimal control problem includes multiple variational inequalities of the form

$$-\Delta\varphi_{i+1} + a_{i+1} - \mu_{i+1} - \kappa\varphi_i = 0, \tag{3.13}$$

with $a_{i+1} \in \partial\Psi_0(\varphi_{i+1})$, which can be reformulated as

$$\langle -\Delta\varphi_{i+1} - \mu_{i+1} - \kappa\varphi_i, \phi - \varphi_{i+1}\rangle \geq 0, \ \forall\phi \in \mathbb{K}. \tag{3.14}$$

As a result the problem (P_Ψ) falls into the realm of mathematical programs with equilibrium constraints in function space, which is well-known for its constraint degeneracy even in finite dimensions. In particular, we have seen in Section 1.6 that, due to the presence of the variational inequality constraint, classical constraint qualifications fail which prevents the application of Karush-Kuhn-Tucker theory for the first-order characterization of optimal solutions by (Lagrange) multipliers.

In order to align with the notation of Section 1.6 we point out that Lemma 2.2.2 ensures that the order parameter φ_{i+1} is an element of $H^2(\Omega)$. Although the subdifferential $\partial\Psi_0$ is in general only contained in the dual space $\overline{H}^1(\Omega)^*$, this allows us to deduce the following additional regularity for the subgradient a_{i+1}

$$a_{i+1} = \Delta\varphi_{i+1} + \mu_{i+1} + \kappa\varphi_i \in L^2(\Omega). \tag{3.15}$$

Consequently, the duality pairing in (3.14) can be equivalently defined as the inner product in $L^2(\Omega)$. Moreover, the following sets are well-defined.

Definition 3.3.1. *For a solution φ_{i+1} of the variational inequality* (3.14)*, we introduce the active sets*

$$\mathscr{A}_{\varphi_{i+1},1} := \{x \in \Omega : \varphi_{i+1}(x) = \psi_1\}, \tag{3.16}$$
$$\mathscr{A}_{\varphi_{i+1},2} := \{x \in \Omega : \varphi_{i+1}(x) = \psi_2\}, \tag{3.17}$$

the strongly active sets

$$\mathscr{A}^+_{\varphi_{i+1},1} := \{x \in \Omega : \varphi_{i+1}(x) = \psi_1 \wedge a^-_{i+1}(x) > 0\}, \tag{3.18}$$
$$\mathscr{A}^+_{\varphi_{i+1},2} := \{x \in \Omega : \varphi_{i+1}(x) = \psi_2 \wedge a^+_{i+1}(x) > 0\}, \tag{3.19}$$

the biactive sets

$$\mathscr{A}^0_{\varphi_{i+1},1} := \{x \in \Omega : \varphi_{i+1}(x) = \psi_1 \wedge a_{i+1}(x) = 0\}, \tag{3.20}$$
$$\mathscr{A}^0_{\varphi_{i+1},2} := \{x \in \Omega : \varphi_{i+1}(x) = \psi_2 \wedge a_{i+1}(x) = 0\}, \tag{3.21}$$

and the inactive set

$$\mathscr{I}_{\varphi_{i+1}} := \{x \in \Omega : \psi_1 < \varphi_{i+1}(x) < \psi_2\} \tag{3.22}$$

Here, $a^+_{i+1}(x) := \max(0, a_{i+1}(x))$ *and* $a^-_{i+1}(x) := -\min(0, a_{i+1}(x))$ *are defined pointwise almost everywhere on* Ω *such that* $a_{i+1} = a^+_{i+1} - a^-_{i+1}$. *Clearly, it holds that*

$$\mathscr{A}^+_{\varphi_{i+1},j} \cup \mathscr{A}^0_{\varphi_{i+1},j} = \mathscr{A}_{\varphi_{i+1},j}, \quad j \in \{1,2\}. \tag{3.23}$$

Note that the variational inequality (3.14) corresponds to the necessary and sufficient first-order optimality condition of the convex optimization problem

$$\min_{\varphi_{i+1} \in \mathbb{K}} \|\nabla \varphi_{i+1}\|^2 - (\mu_{i+1} + \kappa \varphi_i, \varphi_{i+1}). \tag{3.24}$$

In this setting, a^-_{i+1} and a^+_{i+1} correspond to the Lagrange multipliers associated with the inequality constraints $\varphi_{i+1} \geq \psi_1$ and $\varphi_{i+1} \leq \psi_2$, respectively. As discussed in Chapter 1, the variational inequality can be further expressed as the subsequent complementarity system

$$-\Delta \varphi_{i+1} + a_{i+1} - \mu_{i+1} - \kappa \varphi_i = 0, \tag{3.25a}$$
$$\varphi_{i+1} \geq \psi_1, \quad a^-_{i+1} \geq 0, \quad \left(a^-_{i+1}, \varphi_{i+1} - \psi_1\right) = 0, \tag{3.25b}$$
$$\varphi_{i+1} \leq \psi_2, \quad a^+_{i+1} \geq 0, \quad \left(a^+_{i+1}, \varphi_{i+1} - \psi_2\right) = 0. \tag{3.25c}$$

From the complementarity conditions (3.25b), (3.25c), we directly infer that

$$\mathscr{A}_{\varphi_{i+1},1} \cup \mathscr{A}_{\varphi_{i+1},2} \cup \mathscr{I}_{\varphi_{i+1}} = \Omega. \tag{3.26}$$

With the help of (3.25) the optimization problem (P_Ψ) can be equivalently reformulated as the following mathematical program with complementarity conditions

$$
\begin{aligned}
\min \mathscr{J}(\varphi,\mu,v,u) \text{ over } (\varphi,\mu,v,u) &\in \mathscr{X} && \text{(3.27a)}\\
\text{s.t. } u &\in U_{ad}, && \text{(3.27b)}\\
\left\langle \frac{\varphi_{i+1}-\varphi_i}{\tau},\phi \right\rangle + \langle v_{i+1}\nabla\varphi_i,\phi\rangle + (m(\varphi_i)\nabla\mu_{i+1},\nabla\phi) &= 0, && \text{(3.27c)}\\
(\nabla\varphi_{i+1},\nabla\phi) + \langle a_{i+1},\phi\rangle - \langle\mu_{i+1},\phi\rangle - \langle\kappa\varphi_i,\phi\rangle &= 0, && \text{(3.27d)}\\
\varphi_{i+1}\geq\psi_1,\quad a^-_{i+1}\geq 0,\quad \left(a^-_{i+1},\varphi_{i+1}-\psi_1\right) &= 0, && \text{(3.27e)}\\
\varphi_{i+1}\leq\psi_2,\quad a^+_{i+1}\geq 0,\quad \left(a^+_{i+1},\varphi_{i+1}-\psi_2\right) &= 0, && \text{(3.27f)}\\
\left\langle \frac{\rho(\varphi_i)v_{i+1}-\rho(\varphi_{i-1})v_i}{\tau},\psi \right\rangle_{H^{-1}_{0,\sigma},H^1_{0,\sigma}} &- (v_{i+1}\otimes\rho(\varphi_{i-1})v_i,\nabla\psi) \\
+\left(v_{i+1}\otimes\frac{\rho_2-\rho_1}{2}m(\varphi_{i-1})\nabla\mu_i,\nabla\psi\right) &+ (2\eta(\varphi_i)\varepsilon(v_{i+1}),\varepsilon(\psi)) \\
-\langle\mu_{i+1}\nabla\varphi_i,\psi\rangle_{H^{-1}_{0,\sigma},H^1_{0,\sigma}} - \langle u_{i+1},\psi\rangle_{H^{-1}_{0,\sigma},H^1_{0,\sigma}} &= 0, && \text{(3.27g)}
\end{aligned}
$$

where (3.27c)-(3.27f) hold for every $\phi\in\overline{H}^1(\Omega)$, $0\leq i+1\leq M-1$, and equation (3.27g) holds for every $\psi\in H^1_{0,\sigma}(\Omega;\mathbb{R}^N)$, $1\leq i+1\leq M-1$.

In general, the corresponding control-to-state operator S_Ψ is not Fréchet differentiable at u, if the biactive set $\mathscr{A}^0_{\varphi_i,1}\cup\mathscr{A}^0_{\varphi_i,2}$ associated with the state $(\varphi,\mu,v)=S(u)$ is non-empty. Moreover, the feasible set

$$
\{(\varphi,\mu,v,u)\in\mathscr{X} : u\in U_{ad}, (\varphi,\mu,v)=S_\Psi(u)\} \tag{3.28}
$$

is non-convex. Similar to the finite dimensional case discussed in Section 1.6, this gives rise to a hierarchy of stationarity concepts for the problem (3.27).

In order to elaborate on these concepts, we define the associated MPCC-Lagrangian introduced in (1.105).

Definition 3.3.2. *The MPCC-Lagrangian $L:\mathscr{Y}\to\mathbb{R}$ corresponding to (P_Ψ) defined on the product space*

$$
\begin{aligned}
\mathscr{Y} := \overline{H}^1(\Omega)^M\times\overline{H}^1(\Omega)^M\times H^1_{0,\sigma}(\Omega;\mathbb{R}^N)^{M-1}\times\overline{L}^2(\Omega)^M\times L^2(\Omega;\mathbb{R}^n)^{M-1}\\
\times\overline{H}^1(\Omega)^M\times\overline{H}^1(\Omega)^M\times H^1_{0,\sigma}(\Omega;\mathbb{R}^N)^{M-1}\times\overline{H}^1(\Omega)^M\\
\times\left(\overline{H}^1(\Omega)^*\right)^M\times\left(\overline{H}^1(\Omega)^*\right)^M
\end{aligned}
$$

is given by

$$
\begin{aligned}
&L(\varphi,\mu,v,a,u,p,r,q,\pi,\lambda^+,\lambda^-) := \mathscr{J}(\varphi,\mu,v,u) \\
&+\sum_{i=-1}^{M-2}\left[\left\langle \frac{\varphi^{i+1}-\varphi^i}{\tau}, p^{i+1}\right\rangle + \left\langle v^{i+1}\nabla\varphi^i, p^{i+1}\right\rangle + \left\langle m(\varphi^i)\nabla\mu^{i+1}, \nabla p^{i+1}\right\rangle\right] \\
&+\sum_{i=-1}^{M-2}\left[\left\langle -\Delta\varphi^{i+1}, r^{i+1}\right\rangle + \left\langle a^{i+1}, r^{i+1}\right\rangle - \left\langle \mu^{i+1}, r^{i+1}\right\rangle - \left\langle \kappa\varphi^i, r^{i+1}\right\rangle\right] \\
&+\sum_{i=0}^{M-2}\left[\left\langle \frac{\rho(\varphi^i)v^{i+1}-\rho(\varphi^{i+1})v^i}{\tau}, q^{i+1}\right\rangle_{H^{-1}_{0,\sigma},H^1_{0,\sigma}}\right. \\
&-\left(v^{i+1}\otimes\rho(\varphi^{i+1})v^i, \nabla q^{i+1}\right) + \left(v^{i+1}\otimes\frac{\rho_2-\rho_1}{2}m(\varphi^{i+1})\nabla\mu^i, \nabla q^{i+1}\right) \\
&\left.+(2\eta(\varphi^i)\varepsilon(v^{i+1}), \varepsilon(q^{i+1})) - \left\langle \mu^{i+1}\nabla\varphi^i + u^{i+1}, q^{i+1}\right\rangle_{H^{-1}_{0,\sigma},H^1_{0,\sigma}}\right] \\
&-\sum_{i=0}^{M-1}\left\langle a^i, \pi^i\right\rangle + \sum_{i=0}^{M-1}\left\langle (\lambda^i)^+, \varphi^i-\psi_2\right\rangle - \sum_{i=0}^{M-1}\left\langle (\lambda^i)^-, \varphi^i-\psi_1\right\rangle.
\end{aligned}
\tag{3.29}
$$

In general, dual stationarity conditions for a feasible point (φ,μ,v,a,u) of the problem (3.27) are based on the existence of multipliers $(p,r,q,\pi,\lambda^+,\lambda^-)$ such that

$$
\nabla_{(\varphi,\mu,v,a,u)}L[\varphi,\mu,v,a,u,p,r,q,\pi,\lambda^+,\lambda^-](\varphi^\delta,\mu^\delta,v^\delta,a^\delta,u^\delta) = 0, \tag{3.30}
$$

for every direction $(\varphi^\delta,\mu^\delta,v^\delta,a^\delta,u^\delta)$. This leads to the system

$$
\begin{aligned}
&-\frac{1}{\tau}(p^{i+1}-p^i) + m'(\varphi^i)\nabla\mu^{i+1}\cdot\nabla p^{i+1} - \operatorname{div}(p^{i+1}v^{i+1}) - \Delta r^i \\
&+(\lambda^i)^+ - (\lambda^i)^- - \kappa r^{i+2} - \frac{1}{\tau}\rho(\varphi^i)'v^{i+1}\cdot(q^{i+2}-q^{i+1}) \\
&-(\rho(\varphi^i)'v^{i+1} - \frac{\rho_2-\rho_1}{2}m'(\varphi^i)\nabla\mu^{i+1})(Dq^{i+2})^\top v^{i+2} \\
&+2\eta(\varphi^i)'\varepsilon(v^{i+1}) : Dq^{i+1} + \operatorname{div}(\mu^{i+1}q^{i+1}) \;=\; \frac{\partial\mathscr{J}}{\partial\varphi^i}(z),
\end{aligned}
\tag{3.31a}
$$

$$
\begin{aligned}
-r^i - \mathrm{div}(m(\varphi^{i-1})\nabla p^i) - \mathrm{div}(\frac{\rho_2-\rho_1}{2}m(\varphi^{i-1})(Dq^{i+1})^\top v^{i+1})& \\
-q^i\cdot\nabla\varphi^{i-1} &= \frac{\partial \mathscr{J}}{\partial \mu^i}(z),
\end{aligned} \tag{3.31b}
$$

$$
\begin{aligned}
-\frac{1}{\tau}\rho(\varphi^{i-1})(q^{i+1}-q^i) - \rho(\varphi^{i-1})(Dq^{i+1})^\top v^{i+1}& \\
-(Dq^i)(\rho(\varphi^{i-2})v^{i-1} - \frac{\rho_2-\rho_1}{2}m(\varphi^{i-2})\nabla\mu^{i-1})& \\
-\mathrm{div}(2\eta(\varphi^{i-1})\varepsilon(q^i)) + p^i\nabla\varphi^{i-1} &= \frac{\partial \mathscr{J}}{\partial v^i}(z),
\end{aligned} \tag{3.31c}
$$

$$
q^i = \frac{\partial \mathscr{J}}{\partial u^i}(z), \tag{3.31d}
$$

$$
r^i - \pi^i = 0. \tag{3.31e}
$$

Here, we assumed that $U_{ad} = L^2(\Omega;\mathbb{R}^n)^{M-1}$ for the sake of simplicity. A rigorous derivation of the system (3.31) is postponed to the subsequent chapter.

Following the notation of the optimal control of partial differential equations, we refer to the equations (3.31a)-(3.31c) as adjoint equations and call (p,r,q) the corresponding adjoint state. Moreover, the multiplier π can be replaced by the adjoint state r via (3.31e) without loss of information.

As for the finite dimensional problem, the multiplier $r_i(=\pi_i)$ should vanish on the strongly active set $\mathscr{A}^+_{\varphi_i,1}\cup\mathscr{A}^+_{\varphi_i,2}$. Since r_i is an element of $H^1(\Omega)$, the condition can be interpreted pointwise almost everywhere on Ω, i.e.

$$
r_i = 0 \text{ a.e. on } \mathscr{A}^+_{\varphi_i,1}\cup\mathscr{A}^+_{\varphi_i,2}. \tag{3.32}
$$

By the definition of $\mathscr{A}^+_{\varphi_i,1}$, $\mathscr{A}^+_{\varphi_i,2}$, this yields

$$
\langle a_i,\pi_i\rangle = 0. \tag{3.33}
$$

Similarly, we expect the multiplier $\lambda^i := (\lambda^i)^+ - (\lambda^i)^-$ to vanish on the inactive sets $\mathscr{I}_{\varphi_i}$. However, λ_i is in general only contained in $\overline{H}^1(\Omega)^*$ and lacks a pointwise interpretation on Ω. Therefore, it is unclear how to translate the condition to the infinite dimensional setting. Subsequently, we present three possible interpretations, which are connected to different stationarity conditions for the problem (3.27).

Definition 3.3.3. *A point $(\varphi,\mu,v,a,u,p,r,q,\pi,\lambda^+,\lambda^-)\in\mathscr{Y}$ is called weakly stationary for* (3.27)*, if the following conditions are satisfied:*

(I) the point (φ,μ,v,a,u) is feasible, i.e. it fulfills (3.27b)-(3.27g)*;*

(II) the adjoint system (3.31a)-(3.31d) *is satisfied;*

(III) the equality (3.32) *holds true;*

(IV) for every $\phi \in \overline{H}^1(\Omega)$ *with* $\phi|_{\Omega\setminus\mathscr{I}_{\varphi_i}} = 0$ *it holds that*

$$\langle \lambda^i, \phi \rangle = 0. \tag{3.34}$$

It is further called almost weakly stationary, if conditions (I)-(III) are fulfilled and for every $\phi \in \overline{H}^1(\Omega)$ *with* $\phi|_{\Omega\setminus\mathscr{I}_{\varphi_i}} = 0$ *and* $\phi_{|\mathscr{I}_{\varphi_i}} \in H_0^1(\mathscr{I}_{\varphi_i})$ *it holds that*

$$\langle \lambda^i, \phi \rangle = 0, \tag{3.35}$$

$$\big\langle (\lambda^i)^+, \varphi^i - \psi_2 \big\rangle = \big\langle (\lambda^i)^-, \varphi^i - \psi_1 \big\rangle = 0. \tag{3.36}$$

It is called $\mathscr{E}$*-almost weakly stationary, if conditions (I)-(III) are fulfilled and for every* $\varepsilon > 0$ *there exist a measurable subset* $\mathscr{I}_\varepsilon^i$ *of* $\mathscr{I}_{\varphi_i}$ *with* $|\mathscr{I}_{\varphi_i} \setminus \mathscr{I}_\varepsilon^i| < c$ *and*

$$\langle \lambda^i, \phi \rangle = 0 \qquad \forall \phi \in \overline{H}^1(\Omega),\ \ \phi|_{\Omega\setminus\mathscr{I}_\varepsilon^i} = 0, \tag{3.37}$$

$$\big\langle (\lambda^i)^+, \varphi^i - \psi_2 \big\rangle = \big\langle (\lambda^i)^-, \varphi^i - \psi_1 \big\rangle = 0. \tag{3.38}$$

The notion of '$\mathscr{E}$-almost' is motivated by the fact that the proof of the associated stationarity conditions is usually based on the application of Egorov's theorem, cf. e.g. [18].

It can be easily verified that the above weak stationarity concepts obey a hierarchical structure, cf. e.g. [111]. More precisely, every weak stationary point is almost weak stationary and every almost weak stationary point is $\mathscr{E}$-almost weak stationary. The converse is generally not true. However, if the inactive set $\mathscr{I}_{\varphi_i}$ has a Lipschitz boundary, i.e. it possesses the $C^{0,1}$-regularity property from Definition 1.2.1, then the concepts of weak stationarity and almost weak stationarity coincide. Moreover, if λ_i can be defined pointwise almost everywhere on Ω (e.g. if $\lambda_i \in L^1(\Omega)$), then the three concepts are equivalent.

We further note that the equality (3.36) is implied by the definition of weak stationarity due to equation (3.34). Nevertheless it has to be explicitly included for the weaker versions of weak stationarity for which it is no longer automatically satisfied.

The notion of weak stationarity is the weakest available dual stationarity concept in function spaces, as it provides no information on the signs of the multipliers $r_i(=\pi_i)$ and λ_i. Similar to the finite dimensional setting (cf. Section 1.6), however, the above stationarity conditions can be supplemented by a sign condition for the product of r_i and λ_i to form C-stationarity type systems, or paired with explicit conditions for signs of r_i and λ_i, individually, leading to the respective strong stationarity concepts.

In Chapter 4, we establish an infinite-dimensional version of C-stationarity for the problem (P_Ψ), which is associated with the $\mathscr{E}$-almost stationarity concept of Definition 3.3.3. Chapter 5 is devoted to the derivation of strong stationarity conditions for the corresponding unconstrained control problem, i.e. $U_{ad} = L^2(\Omega;\mathbb{R}^n)^{M-1}$, based on a suitable characterization of the involved directional derivatives.

Our theoretical studies are accompanied by a thorough analysis and implementation of related numerical solution methods. A penalization algorithm, which computes an $\mathscr{E}$-almost C-stationary point, is considered in Chapter 4, whereas Chapter 5 elaborates on a bundle-free implicit programming approach targeting strong stationary points of the optimal control problem.

Chapter 4

$\mathscr{E}$-almost C-stationarity conditions

4.1 A smooth penalization approach

This section is concerned with derivation of $\mathscr{E}$-almost C-stationarity conditions for the optimal control problem (P_Ψ) associated with the double-obstacle potential. For this purpose, a Yosida regularization technique is applied, which is reminiscent of the one pioneered by Barbu in [18]. More precisely, we approximate the problem (P_Ψ) by nonlinear auxiliary programs, where the double-obstacle is replaced by certain double-well type potentials satisfying Assumption 2.1.2, (II). These potentials correspond to Moreau–Yosida type approximations of the double-obstacle potential.

In Subsection 4.1.1, necessary first-order optimality conditions for the nonlinear auxiliary programs are established by means of classical optimization theory in Banach spaces. In particular, we employ Theorem 1.3.5. This is followed by a careful analysis of the limit process with respect to the Yosida parameter leading to a C-stationarity system for the double-obstacle potential in Subsection 4.1.2.

Assumption 4.1.1. *In the sequel, we consider a sequence of potentials* $\left\{\Psi^{(k)}\right\}_{k\in\mathbb{N}}$ *such that*

(I) Assumption 2.1.2, (II) is satisfied for every $k \in \mathbb{N}$*;*

(II) for every strongly convergent sequence

$$(x^{(k)}, y^{(k)}) \to (x^{(\infty)}, y^{(\infty)}) \text{ in } \overline{H}^1(\Omega) \times \overline{H}^1(\Omega)^* \tag{4.1}$$

with $y^{(k)} = \Psi^{(k)\prime}(x^{(k)})$ *it holds that*

$$y^{(\infty)} \in \partial\overline{\Psi}(x^{(\infty)}), \tag{4.2}$$

where $\overline{\Psi}$ *denotes the double-obstacle potential from* (2.40).

Condition (4.2) serves as a mathematical reflection of the approximation properties of the regularized potentials. We point out that the results of the preceding sections, in particular, Theorem 2.2.1 and Theorem 2.2.3, already ensure the existence of global solutions to the auxiliary problems associated with the potentials $\Psi^{(k)}$, $k \in \mathbb{N}$.

The next theorem verifies the consistency of the regularization method, i.e. the convergence of a sequence of globally optimal points of $(P_{\Psi^{(k)}})$ to a global solution of $(P_{\overline{\Psi}})$ for $k \to \infty$.

Theorem 4.1.1 (Consistency of the regularization)**.** *Assume that the function*

$$\mathscr{J} : \overline{H}^1(\Omega)^M \times \overline{H}^1(\Omega)^M \times H^1_{0,\sigma}(\Omega;\mathbb{R}^N)^{M-1} \times L^2(\Omega;\mathbb{R}^N)^{M-1} \to \mathbb{R} \tag{4.3}$$

is upper-semicontinuous and let

$$\left\{(\varphi^{(k)},\mu^{(k)},v^{(k)},u^{(k)})\right\}_{k\in\mathbb{N}}\subset\overline{H}^2(\Omega)^M\times\overline{H}^2(\Omega)^M\times H^1_{0,\sigma}(\Omega;\mathbb{R}^N)^{M-1}\times U_{ad} \tag{4.4}$$

be a sequence of global solutions to ($P_{\Psi^{(k)}}$). If U_{ad} is unbounded, then we additionally suppose that $\left\{\mathscr{J}(\varphi^{(k)},\mu^{(k)},v^{(k)},u^{(k)})\right\}_{k\in\mathbb{N}}$ is bounded.

Then the sequence $\left\{(\varphi^{(k)},\mu^{(k)},v^{(k)},u^{(k)})\right\}_{k\in\mathbb{N}}$ converges strongly to a global solution of ($P_{\overline{\Psi}}$) in $\overline{H}^1(\Omega)^M\times\overline{H}^1(\Omega)^M\times H^1_{0,\sigma}(\Omega;\mathbb{R}^N)^{M-1}\times L^2(\Omega;\mathbb{R}^N)^{M-1}$.

Proof. First note that the sequence $\left\{u^{(k)}\right\}_{k\in\mathbb{N}}$ is bounded in the reflexive Banach space $L^2(\Omega;\mathbb{R}^N)^{M-1}$, which follows either from the boundedness of the set U_{ad} or from the partial coercivity of $\mathscr{J}$ combined with the boundedness of $\left\{\mathscr{J}(\varphi^{(k)},\mu^{(k)},v^{(k)},u^{(k)})\right\}_{k\in\mathbb{N}}$ in $\mathbb{R}$.

Employing Lemma 2.2.4, we secure the boundedness of $\left\{(\varphi^{(k)},\mu^{(k)},v^{(k)})\right\}_{k\in\mathbb{N}}$ in $\overline{H}^2_{\partial_n}(\Omega)^M\times\overline{H}^2_{\partial_n}(\Omega)^M\times H^1_{0,\sigma}(\Omega;\mathbb{R}^N)^{M-1}$. Hence there exists a weakly convergent sequence

$$\left\{w^{(k_l)}\right\}_{l\in\mathbb{N}}:=\left\{(\varphi^{(k_l)},\mu^{(k_l)},v^{(k_l)},u^{(k_l)})\right\}_{l\in\mathbb{N}} \tag{4.5}$$

with limit point

$$\overline{w}:=(\overline{\varphi},\overline{\mu},\overline{v},\overline{u})\in\overline{H}^2_{\partial_n}(\Omega)^M\times\overline{H}^2_{\partial_n}(\Omega)^M\times H^1_{0,\sigma}(\Omega;\mathbb{R}^N)^{M-1}. \tag{4.6}$$

Since U_{ad} is weakly closed, $\overline{u}$ belongs to U_{ad}.

Following the argumentation of Theorem 3.2.1, it is shown that the limit point satisfies the semi-discrete Cahn–Hilliard–Navier–Stokes system, i.e. $(\overline{\varphi},\overline{\mu},\overline{v})\in S_{\overline{\Psi}}(\overline{u})$. The only difference is that inclusion (3.12) is inferred from condition (4.2) (instead of the maximal monotonicity of the potential).

Next, we prove that $\overline{w}$ is an optimal point of ($P_{\overline{\Psi}}$). For this purpose, we consider an arbitrary optimal solution $(\widehat{\varphi},\widehat{\mu},\widehat{v},\widehat{u})$ of ($P_{\overline{\Psi}}$) and a corresponding sequence $(\widehat{\varphi}^{(k)},\widehat{\mu}^{(k)})\in\overline{H}^2_{\partial_n}(\Omega)^M\times\overline{H}^2_{\partial_n}(\Omega)^M$ such that

$$\left\langle\frac{\widehat{\varphi}^{(k)}_{i+1}-\widehat{\varphi}^{(k)}_i}{\tau},\phi\right\rangle+\left\langle\widehat{v}_{i+1}\nabla\widehat{\varphi}^{(k)}_i,\phi\right\rangle+\left\langle m(\widehat{\varphi}^{(k)}_i)\nabla\widehat{\mu}^{(k)}_{i+1},\nabla\phi\right\rangle=0, \tag{4.7}$$

$$\left\langle\nabla\widehat{\varphi}^{(k)}_{i+1},\nabla\phi\right\rangle+\left\langle\left(\Psi^{(k)}_0\right)'(\widehat{\varphi}^{(k)}_{i+1}),\phi\right\rangle-\left\langle\widehat{\mu}^{(k)}_{i+1},\phi\right\rangle-\left\langle\kappa\widehat{\varphi}^{(k)}_i,\phi\right\rangle=0, \tag{4.8}$$

for every $\phi \in \overline{H}^1(\Omega)$ and $i \in \{-1,..,M-2\}$. Note that the operator $L_a^{(k)} : \overline{H}^1(\Omega) \times \overline{H}^1(\Omega) \to \overline{H}^1(\Omega)^* \times \overline{H}^1(\Omega)^*$ defined by

$$L_a^{(k)}(\varphi,\mu) := \left(-\Delta\varphi + \left(\Psi_0^{(k)}\right)'(\varphi) - \mu, \varphi - \operatorname{div}(a\nabla\mu)\right) \tag{4.9}$$

is monotone, coercive and continuous, if $a \in H^2(\Omega)$ satisfies $0 < \tau b_1 \leq a(x) \leq \tau b_2$ almost everywhere on Ω. Hence for fixed $k \in \mathbb{N}$, the pair $(\widehat{\varphi}_{i+1}^{(k)}, \widehat{\mu}_{i+1}^{(k)})$ of each subsequent time step is uniquely determined as the solution to

$$L^{(k)}_{m(\widehat{\varphi}_i^{(k)})\tau}(\widehat{\varphi}_{i+1}^{(k)}, \widehat{\mu}_{i+1}^{(k)}) = (\kappa\widehat{\varphi}_i^{(k)}, \widehat{\varphi}_i^{(k)} - \tau\widehat{v}_{i+1}\nabla\widehat{\varphi}_i^{(k)}), \tag{4.10}$$

where

$$0 < \tau b_1 \leq a := m(\widehat{\varphi}_i^{(k)})h \leq \tau b_2 \quad \text{ a.e. on } \Omega \tag{4.11}$$

cf. [175, Chapter II, Theorem 2.2]. Due to Lemma 2.2.2, $(\widehat{\varphi}^{(k)}, \widehat{\mu}^{(k)}, \widehat{v})_{k\in\mathbb{N}}$ is bounded in $\overline{H}^2(\Omega)^M \times \overline{H}^2(\Omega)^M \times H^1_{0,\sigma}(\Omega;\mathbb{R}^N)^{M-1}$. Consequently, there exists a subsequence (denoted the same) which converges weakly to a limit point $(\widehat{\varphi}^*, \widehat{\mu}^*, \widehat{v})$.

In accordance with the above observations and due to condition (4.2), the limit point $(\widehat{\varphi}_{i+1}^*, \widehat{\mu}_{i+1}^*)$ is the unique solution to the system

$$\left\langle \frac{\widehat{\varphi}_{i+1}^* - \widehat{\varphi}_i^*}{\tau}, \phi \right\rangle + \langle \widehat{v}_{i+1}\nabla\widehat{\varphi}_i^*, \phi\rangle + \left\langle m(\widehat{\varphi}_i^*)\nabla\widehat{\mu}_{i+1}^*, \nabla\phi\right\rangle = 0,\ \forall\phi \in \overline{H}^1(\Omega), \tag{4.12}$$

$$\left\langle \nabla\widehat{\varphi}_{i+1}^*, \nabla\phi\right\rangle + \left\langle \partial\overline{\Psi}_0(\widehat{\varphi}_{i+1}^*), \phi\right\rangle - \left\langle \widehat{\mu}_{i+1}^*, \phi\right\rangle - \langle \kappa\widehat{\varphi}_i^*, \phi\rangle = 0,\ \forall\phi \in \overline{H}^1(\Omega), \tag{4.13}$$

for every $i \in \{-1,..,M-2\}$. Since $(\widehat{\varphi}, \widehat{\mu}, \widehat{v}, \widehat{u})$ is a feasible point for the optimal control problem $(P_{\overline{\Psi}})$ it holds that $(\widehat{\varphi}, \widehat{\mu}, \widehat{v}) \in S_{\overline{\Psi}}(\widehat{u})$. In particular, $(\widehat{\varphi}, \widehat{\mu})$ also solves the system (4.12)-(4.13), which implies $\widehat{\varphi}^* = \widehat{\varphi}$ and $\widehat{\mu}^* = \widehat{\mu}$.

Our next goal is to show the strong convergence of $\widehat{\mu}^{(k)} \to \widehat{\mu}^*$ in $(\overline{H}^2_{\partial_n}(\Omega))^M$. For this purpose, we fix $i \in \{-1,..,M-2\}$ and define

$$g_i^{(k)} := \frac{\widehat{\varphi}_{i+1}^{(k)} - \widehat{\varphi}_i^{(k)}}{\tau} + \widehat{v}_{i+1}\nabla\widehat{\varphi}_i^{(k)}, \quad g_i^* := \frac{\widehat{\varphi}_{i+1}^* - \widehat{\varphi}_i^*}{\tau} + \widehat{v}_{i+1}\nabla\widehat{\varphi}_i^*. \tag{4.14}$$

By the Rellich-Kondrachov theorem $g_i^{(k)}$ converges strongly in $L^2(\Omega)$ to g_i^*. It further holds that

$$g_i^{(k)} - g_i^* = \operatorname{div}(m(\widehat{\varphi}_i^{(k)})\nabla\widehat{\mu}_{i+1}^{(k)}) - \operatorname{div}(m(\widehat{\varphi}_i^*)\nabla\widehat{\mu}_{i+1}^*). \tag{4.15}$$

Hence, we have

$$\begin{aligned}\operatorname{div}(m(\widehat{\varphi}_i^*)\nabla(\widehat{\mu}_{i+1}^{(k)}-\widehat{\mu}_{i+1}^*)) =& g_i^{(k)}-g_i^*-\operatorname{div}((m(\widehat{\varphi}_i^{(k)})-m(\widehat{\varphi}_i^*))\nabla\widehat{\mu}_{i+1}^{(k)})\\ =&:\delta_i^{(k)}.\end{aligned}$$

Again by the Rellich-Kondrachov theorem $m(\widehat{\varphi}_i^{(k)})$ converges strongly to $m(\widehat{\varphi}_i^*)$ in $W^{1,5}(\Omega)$. Furthermore, $\nabla\widehat{\mu}_{i+1}^{(k)}$ is bounded in $H^1(\Omega)$. As a consequence, $\delta_i^{(k)}$ tends to zero in $L^2(\Omega)$.

Applying [144, Theorem 2.3.1], we conclude

$$\left\|\widehat{\mu}_{i+1}^{(k)}-\widehat{\mu}_{i+1}^*\right\|_{H^2}\leq C\left\|\delta_i^{(k)}\right\|\to 0.$$

Next, we define $\widehat{u}_{i+1}^{(k)}\in L^2(\Omega;\mathbb{R}^N)$ for all $i\in\{0,..,M-2\}$ by

$$\begin{aligned}\widehat{u}_{i+1}^{(k)}:=&\frac{\rho(\widehat{\varphi}_i^{(k)})\widehat{v}_{i+1}-\rho(\widehat{\varphi}_{i-1}^{(k)})\widehat{v}_i}{\tau}+\operatorname{div}(\widehat{v}_{i+1}\otimes\rho(\widehat{\varphi}_{i-1}^{(k)})\widehat{v}_i)\\ &-\operatorname{div}(\widehat{v}_{i+1}\otimes\frac{\rho_2-\rho_1}{2}m(\widehat{\varphi}_{i-1}^{(k)})\nabla\widehat{\mu}_i^{(k)})\\ &-\operatorname{div}(2\eta(\widehat{\varphi}_i^{(k)})\varepsilon(\widehat{v}_{i+1}))-\widehat{\mu}_{i+1}^{(k)}\nabla\widehat{\varphi}_i^{(k)}.\end{aligned}$$

Similarly to the proof of Theorem 3.2.1, it can be shown that $\widehat{u}^{(k)}$ converges strongly in $L^2(\Omega;\mathbb{R}^N)^{M-1}$ to $\widehat{u}$.

In summary, it has been shown that the sequence

$$\left(\widehat{\varphi}^{(k)},\widehat{\mu}^{(k)},\widehat{v},\widehat{u}^{(k)}\right)\to(\widehat{\varphi},\widehat{\mu},\widehat{v},\widehat{u}) \tag{4.16}$$

in $\overline{H}^1(\Omega)^M\times\overline{H}^1(\Omega)^M\times H^1_{0,\sigma}(\Omega;\mathbb{R}^N)^{M-1}\times L^2(\Omega;\mathbb{R}^N)^{M-1}$ for $k\to\infty$.

Employing the continuity properties of the objective functional $\mathscr{J}$, this yields

$$\begin{aligned}\mathscr{J}(\overline{\varphi},\overline{\mu},\overline{v},\overline{u})\leq&\lim_{k\to\infty}\mathscr{J}(\varphi^{(k)},\mu^{(k)},v^{(k)},u^{(k)})\leq\lim_{k\to\infty}\mathscr{J}(\widehat{\varphi}^{(k)},\widehat{\mu}^{(k)},\widehat{v},\widehat{u}^{(k)})\\ \leq&\mathscr{J}(\widehat{\varphi},\widehat{\mu},\widehat{v},\widehat{u}).\end{aligned}\tag{4.17}$$

Since $(\widehat{\varphi},\widehat{\mu},\widehat{v},\widehat{u})$ is optimal, the assertion holds true. □

In summary, the optimal control problems under consideration are well-posed and admit globally optimal solutions. Furthermore, the chosen regularization approach is consistent in the sense of Theorem 4.1.1.

4.1.1 Necessary optimality conditions for the smooth free energy potentials

The subsequent theorem derives a necessary first-order optimality system for the nonlinear auxiliary programs associated with $\Psi^{(k)}$. For this purpose, we adopt the notation of [191] and verify that the constraint qualification (1.77) is fulfilled.

Theorem 4.1.2 (Karush-Kuhn-Tucker type optimality conditions)**.** *Let*

$$\mathscr{J} : \overline{H}^1(\Omega)^M \times \overline{H}^1(\Omega)^M \times H^1_{0,\sigma}(\Omega;\mathbb{R}^N)^{M-1} \times L^2(\Omega;\mathbb{R}^N)^{M-1} \to \mathbb{R} \quad (4.18)$$

be Fréchet differentiable and suppose that Ψ_0' maps $\overline{H}^2_{\partial_n}(\Omega)$ continuously Frèchet differentiable into $L^2(\Omega)$.

For a minimizer $\bar{z} := (\bar{\varphi}, \bar{\mu}, \bar{v}, \bar{u})$ of $(P_{\Psi^{(k)}})$, there exist adjoint states

$$(p,r,q) \in \overline{L}^2(\Omega)^M \times \overline{L}^2(\Omega)^M \times H^1_{0,\sigma}(\Omega;\mathbb{R}^N)^{M-1}, \quad (4.19)$$

with $p = (p_{-1}, \ldots p_{M-2})$, $r = (r_{-1}, \ldots r_{M-2})$, $q = (q_0, \ldots q_{M-2})$, such that

$$\begin{aligned}
-\frac{1}{\tau}(p_i - p_{i-1}) + a(m'(\varphi_i), \mu_{i+1}, p_i) - \operatorname{div}(p_i v_{i+1}) - \Delta^t r_{i-1}& \\
+\Psi_0^{(k)''}(\varphi_i)^* r_{i-1} - \kappa r_{i+1} - \frac{1}{\tau}\rho'(\varphi_i) v_{i+1} \cdot (q_{i+1} - q_i)& \\
-(\rho'(\varphi_i) v_{i+1} - \frac{\rho_2 - \rho_1}{2} m'(\varphi_i) \nabla \mu_{i+1})(Dq_{i+1})^\top v_{i+2}& \\
+2\eta'(\varphi_i)\varepsilon(v_{i+1}) : Dq_i + \operatorname{div}(\mu_{i+1} q_i) &= \frac{\partial \mathscr{J}}{\partial \varphi_i}(\bar{z}),
\end{aligned} \quad (4.20)$$

$$\begin{aligned}
-r_{i-1} + b(m(\varphi_{i-1}), p_{i-1}) - \operatorname{div}(\frac{\rho_2 - \rho_1}{2} m(\varphi_{i-1})(Dq_i)^\top v_{i+1})& \\
-q_{i-1} \cdot \nabla \varphi_{i-1} &= \frac{\partial \mathscr{J}}{\partial \mu_i}(\bar{z}),
\end{aligned} \quad (4.21)$$

$$\begin{aligned}
-\frac{1}{\tau}\rho(\varphi_{j-1})(q_j - q_{j-1}) - \rho(\varphi_{j-1})(Dq_j)^\top v_{j+1}& \\
-(Dq_{j-1})(\rho(\varphi_{j-2}) v_{j-1} - \frac{\rho_2 - \rho_1}{2} m(\varphi_{j-2}) \nabla \mu_{j-1})& \\
-\operatorname{div}(2\eta(\varphi_{j-1})\varepsilon(q_{j-1})) + p_{j-1} \nabla \varphi_{j-1} &= \frac{\partial \mathscr{J}}{\partial v_j}(\bar{z}),
\end{aligned} \quad (4.22)$$

$$\Big(\frac{\partial \mathscr{J}}{\partial u_k}(\bar{z}) - q_{k-1}\Big)_{k=1}^{M-1} \in \big[\mathbb{R}_+(U_{ad} - \bar{u})\big]^0, \quad (4.23)$$

for all $i = 0, ..., M-1$ and $j = 1, ..., M-1$.

Here, $\left[\mathbb{R}_+(U_{ad} - \bar{u})\right]^0$ denotes the polar cone of $\{r(w-u) | w \in U_{ad} \wedge r \in \mathbb{R}^+\}$, cf. Definition 1.3.2. Moreover, we employed the following definitions

$$\begin{aligned}
\langle \Delta^t \hat{r}, \hat{z} \rangle &:= \int_\Omega \hat{r} \Delta \hat{z} dx, && (4.24)\\
\langle a(\hat{f}, \hat{w}, \hat{p}), \hat{z} \rangle &:= \int_\Omega -\hat{p} \operatorname{div}(\hat{f} \hat{z} \nabla \hat{w}) dx, && (4.25)\\
\langle b(\hat{m}, \hat{p}), \hat{z} \rangle &:= \int_\Omega -\hat{p} \operatorname{div}(\hat{m} \nabla \hat{z}) dx, && (4.26)
\end{aligned}$$

for functions $\hat{f}, \hat{m} \in C^1(\overline{\Omega}), \hat{w} \in H^1(\Omega), \hat{r}, \hat{p} \in L^2(\Omega)$ and $\hat{z} \in \overline{H}^2_{\partial_n}(\Omega)$.

Finally, we use the convention that p_i, r_i, q_i are equal to 0 for $i \geq M-1$ along with q_{-1} and φ_i, μ_i, v_i for $i \geq M$.

Proof. Utilizing the spaces X and Y and the set C given by

$$\begin{aligned}
X &:= \overline{H}^2_{\partial_n}(\Omega)^M \times \overline{H}^2_{\partial_n}(\Omega)^M \times H^1_{0,\sigma}(\Omega; \mathbb{R}^N)^{M-1} \times L^2(\Omega; \mathbb{R}^N)^{M-1},\\
C &:= \overline{H}^2_{\partial_n}(\Omega)^M \times \overline{H}^2_{\partial_n}(\Omega)^M \times H^1_{0,\sigma}(\Omega; \mathbb{R}^N)^{M-1} \times U_{ad},\\
Y &:= (\overline{L}^2(\Omega))^{*^M} \times (\overline{L}^2(\Omega))^{*^M} \times H^1_{0,\sigma}(\Omega; \mathbb{R}^N)^{*^{M-1}},
\end{aligned}$$

for $\varphi = (\varphi_0, ..., \varphi_{M-1})$, $\mu = (\mu_0, ..., \mu_{M-1})$, $v = (v_1, ..., v_{M-1})$, $u = (u_1, ..., u_{M-1})$, we define the mapping $g : X \to Y$ by

$$g(\varphi, \mu, v, u) :=
\begin{pmatrix}
\left(\frac{1}{\tau}(\varphi_{i+1} - \varphi_i) - \operatorname{div}(m(\varphi_i) \nabla \mu_{i+1}) + v_{i+1} \cdot \nabla \varphi_i \right)_{i=-1}^{M-2} \\
\left(-\mu_{i+1} - \Delta \varphi_{i+1} + \Psi_0^{(k)'}(\varphi_{i+1}) - \kappa \varphi_i \right)_{i=-1}^{M-2} \\
\begin{pmatrix}
\frac{1}{\tau}(\rho(\varphi_i) v_{i+1} - \rho(\varphi_{i-1}) v_i) - \operatorname{div}(2\eta(\varphi_i) \varepsilon(v_{i+1})) \\
+ \operatorname{div}(v_{i+1} \otimes (\rho(\varphi_{i-1}) v_i - \frac{\rho_2 - \rho_1}{2} m(\varphi_{i-1}) \nabla \mu_i)) \\
-\mu_{i+1} \nabla \varphi_i - u_{i+1}
\end{pmatrix}_{i=0}^{M-2}
\end{pmatrix}.$$

Then, the optimal control problem $(P_{\Psi^{(k)}})$ is equivalent to

$$\begin{aligned}
&\min \mathscr{J}(\varphi, \mu, v, u) \text{ over } (\varphi, \mu, v, u) \in C,\\
&\quad \text{s.t. } g(\varphi, \mu, v, u) = 0,
\end{aligned} \tag{4.27}$$

In order to verify that the mapping g is continuously Frèchet differentiable from X into Y, we exemplary consider the term $\operatorname{div}(m(\varphi_i) \nabla \mu_{i+1})$. First note that

$$\operatorname{div}(m(\varphi_i) \nabla \mu_{i+1}) = \nabla m(\varphi_i) \cdot \nabla \mu_{i+1} + m(\varphi_i) \Delta \mu_{i+1}, \tag{4.28}$$

where $\nabla m(\varphi_i) = m'(\varphi_i)\nabla\varphi_i$. Assumption 2.1.1 implies that both superposition operators $\widetilde{\varphi} \mapsto m(\widetilde{\varphi})$, $\widetilde{\varphi} \mapsto m'(\widetilde{\varphi})$ are continuously Frèchet differentiable from $H^2(\Omega) \hookrightarrow L^\infty(\Omega)$ into $L^\infty(\Omega)$ (cf. [182]). Therefore, the mappings

$$(\widetilde{\varphi}, \widetilde{\mu}) \to m'(\widetilde{\varphi})\nabla\widetilde{\varphi}\cdot\nabla\widetilde{\mu} \ : \ H^2(\Omega)\times H^2(\Omega) \to L^3(\Omega), \tag{4.29}$$

$$(\widetilde{\varphi}, \widetilde{\mu}) \to m(\widetilde{\varphi})\Delta\widetilde{\mu} \ : \ H^2(\Omega)\times H^2(\Omega) \to L^2(\Omega), \tag{4.30}$$

are continuously Frèchet differentiable. This shows the continuous Frèchet differentiability of $\operatorname{div}(m(\varphi_i)\nabla\mu_{i+1})$. The other terms appearing in the definition of g can be treated analogously.

Then, the Frèchet derivative of g in (φ,μ,v,u) applied to $(\varphi^\delta,\mu^\delta,v^\delta,u^\delta) \in X$ is given by

$$g'(\varphi,\mu,v,u)(\varphi^\delta,\mu^\delta,v^\delta,u^\delta) =$$
$$\begin{pmatrix} \begin{pmatrix} \frac{1}{\tau}(\varphi_{i+1}^\delta - \varphi_i^\delta) - \operatorname{div}(m'(\varphi_i)\varphi_i^\delta\nabla\mu_{i+1}) - \operatorname{div}(m(\varphi_i)\nabla\mu_{i+1}^\delta) \\ \quad +v_{i+1}\cdot\nabla\varphi_i^\delta + v_{i+1}^\delta\cdot\nabla\varphi_i \end{pmatrix}_{i=-1}^{M-2} \\ \begin{pmatrix} -\mu_{i+1}^\delta - \Delta\varphi_{i+1}^\delta + {\Psi^{(k)}}''_0(\varphi_{i+1};\varphi_{i+1}^\delta) - \kappa\varphi_i^\delta \end{pmatrix}_{i=-1}^{M-2} \\ \begin{pmatrix} \frac{1}{\tau}(\rho'(\varphi_i)\varphi_i^\delta v_{i+1} - \rho'(\varphi_{i-1})\varphi_{i-1}^\delta v_i) \\ \quad +\frac{1}{\tau}(\rho(\varphi_i)v_{i+1}^\delta - \rho(\varphi_{i-1})v_i^\delta) \\ \quad +\operatorname{div}(v_{i+1}\otimes(\rho'(\varphi_{i-1})\varphi_{i-1}^\delta v_i + \rho(\varphi_{i-1})v_i^\delta)) \\ \quad -\operatorname{div}(v_{i+1}\otimes(\frac{\rho_2-\rho_1}{2}m'(\varphi_{i-1})\varphi_{i-1}^\delta\nabla\mu_i)) \\ \quad +\operatorname{div}(v_{i+1}\otimes(\frac{\rho_2-\rho_1}{2}m(\varphi_{i-1})\nabla\mu_i^\delta)) \\ \quad +\operatorname{div}(v_{i+1}^\delta\otimes(\rho(\varphi_{i-1})v_i - \frac{\rho_2-\rho_1}{2}m(\varphi_{i-1})\nabla\mu_i)) \\ \quad -\operatorname{div}(2\eta'(\varphi_i)\varphi_i^\delta\varepsilon(v_{i+1})) - \operatorname{div}(2\eta(\varphi_i)\varepsilon(v_{i+1}^\delta)) \\ \quad -\mu_{i+1}\nabla\varphi_i^\delta - \mu_{i+1}^\delta\nabla\varphi_i - u_{i+1}^\delta \end{pmatrix}_{i=0}^{M-2} \end{pmatrix}.$$

Due to our convention for φ_{-1} and v_0, we require that $\varphi_{-1}^\delta = 0$ and $v_0^\delta = 0$.

For the application of Theorem 1.3.5 to ensure the existence of Lagrange multipliers, we aim to show that

$$\forall y \in Y \ \exists z^\delta \in \mathbb{R}_+(C-\bar{z}) \subset X \ : \ g'[\bar{z}](z^\delta) = y \tag{4.31}$$

For this purpose, let $(\Theta_i^c, \Theta_i^w, \Theta_i^v) \in Y$ be arbitrarily fixed. Then, (4.31) is equivalent to the existence of a tuple $(\varphi^\delta,\mu^\delta,v^\delta,u^\delta)\in\mathbb{R}_+(C-\bar z)$ such that

$$\frac{1}{\tau}(\varphi_{i+1}^\delta-\varphi_i^\delta)-\operatorname{div}(m'(\varphi_i)\varphi_i^\delta\nabla\mu_{i+1})-\operatorname{div}(m(\varphi_i)\nabla\mu_{i+1}^\delta)$$
$$+v_{i+1}\cdot\nabla\varphi_i^\delta+v_{i+1}^\delta\cdot\nabla\varphi_i=\Theta_i^w, \tag{4.32}$$

$$-\mu_{i+1}^\delta-\Delta\varphi_{i+1}^\delta-\kappa\varphi_i^\delta+\Psi_0^{(k)''}(\varphi_{i+1};\varphi_{i+1}^\delta)=\Theta_i^c, \tag{4.33}$$

$$\frac{1}{\tau}(\rho'(\varphi_i)\varphi_i^\delta v_{i+1}-\rho'(\varphi_{i-1})\varphi_{i-1}^\delta v_i)+\frac{1}{\tau}(\rho(\varphi_i)v_{i+1}^\delta-\rho(\varphi_{i-1})v_i^\delta)$$
$$+\operatorname{div}(v_{i+1}\otimes(\rho'(\varphi_{i-1})\varphi_{i-1}^\delta v_i+\rho(\varphi_{i-1})v_i^\delta))$$
$$-\operatorname{div}(v_{i+1}\otimes(\frac{\rho_2-\rho_1}{2}m'(\varphi_{i-1})\varphi_{i-1}^\delta\nabla\mu_i-\frac{\rho_2-\rho_1}{2}m(\varphi_{i-1})\nabla\mu_i^\delta))$$
$$+\operatorname{div}(v_{i+1}^\delta\otimes(\rho(\varphi_{i-1})v_i-\frac{\rho_2-\rho_1}{2}m(\varphi_{i-1})\nabla\mu_i))$$
$$-\operatorname{div}(2\eta'(\varphi_i)\varphi_i^\delta\varepsilon(v_{i+1}))-\operatorname{div}(2\eta(\varphi_i)\varepsilon(v_{i+1}^\delta))$$
$$-\mu_{i+1}\nabla\varphi_i^\delta-\mu_{i+1}^\delta\nabla\varphi_i-u_{i+1}^\delta=\Theta_i^v, \tag{4.34}$$

where (4.32) and (4.33) hold for $i=-1,...,M-2$ and (4.34) for all $i=0,...,M-1$. As in Theorem 2.2.1, standard arguments show the existence of a point $(\varphi_0^\delta,\mu_0^\delta)\in\overline{H}^2_{\partial_n}(\Omega)\times\overline{H}^2_{\partial_n}(\Omega)$ such that (4.32) and (4.33) are fulfilled for $i=-1$.

Now we apply induction over the time step i and assume that (4.32)–(4.34) hold for $i<M-1$. In order to show the existence of a solution to this system for $i+1$, we observe that it can be written as

$$\frac{1}{\tau}(\varphi_{i+2}^\delta-\varphi_{i+1}^\delta)-\operatorname{div}(m(\varphi_{i+1})\nabla\mu_{i+2}^\delta)+v_{i+2}^\delta\cdot\nabla\varphi_{i+1}=\Theta_\mu, \tag{4.35a}$$

$$-\mu_{i+2}^\delta-\Delta\varphi_{i+2}^\delta-\kappa\varphi_{i+1}^\delta+\Psi^{(k)}\varphi_{i+2};\varphi_{i+2}^\delta)=\Theta_\varphi, \tag{4.35b}$$

$$\frac{1}{\tau}(\rho(\varphi_{i+1})v_{i+2}^\delta-\rho(\varphi_i)v_{i+1}^\delta)$$
$$+\operatorname{div}(v_{i+2}^\delta\otimes(\rho(\varphi_i)v_{i+1}-\frac{\rho_2-\rho_1}{2}m(\varphi_i)\nabla\mu_{i+1}))$$
$$-\operatorname{div}(2\eta(\varphi_{i+1})\varepsilon(v_{i+2}^\delta))-\mu_{i+2}^\delta\nabla\varphi_{i+1}-u_{i+2}^\delta=\Theta_v, \tag{4.35c}$$

for a triple $(\Theta_\varphi,\Theta_\mu,\Theta_v)\in(\overline{L}^2(\Omega))^*\times(\overline{L}^2(\Omega))^*\times H^1_{0,\sigma}(\Omega;\mathbb{R}^N)^*$ that only depends on (φ,μ,v), on $\varphi_i^\delta,\mu_i^\delta$ and v_i^δ for $i<M-1$ and on $(\Theta_{i+1}^c,\Theta_{i+1}^w,\Theta_{i+1}^v)$.

The existence of a solution to the system (4.35) follows readily from Theorem 2.2.1 and from Lemma 2.2.2 when choosing

$$v = \rho(\varphi_i)v_{i+1} - \frac{\rho_2-\rho_1}{2}m(\varphi_i)\nabla\mu_{i+1}, f_0 = \rho(\varphi_{i+1}), f_{-1} = \rho(\varphi_i). \quad (4.36)$$

Note that the functions $\rho(\varphi_{i+1}), m(\varphi_{i+1}), \eta(\varphi_{i+1})$ do not depend on the unknown φ_{i+2}^{δ}. Moreover, we can always find a convex, affine functional $\psi : \overline{H}^2_{\partial_n}(\Omega) \mapsto \mathbb{R}$ with $(D\psi)z = \Psi_0^{(k)''}(\varphi_{i+2}; z)$ for all $z \in \overline{H}^2_{\partial_n}(\Omega)$. Hence we deduce the existence of a Lagrange multiplier $(p,r,q) \in Y^*$ such that

$$\begin{aligned} \mathscr{J}'(\bar\varphi,\bar\mu,\bar v,\bar u)(\varphi^\delta,\mu^\delta,v^\delta,u^\delta) &= \langle g'(\bar\varphi,\bar\mu,\bar v,\bar u)(\varphi^\delta,\mu^\delta,v^\delta,u^\delta),(p,r,q)\rangle \\ &= \langle g'(\bar\varphi,\bar\mu,\bar v,\bar u)^*(p,r,q),(\varphi^\delta,\mu^\delta,v^\delta,u^\delta)\rangle, \end{aligned} \quad (4.37)$$

for all $(\varphi^\delta,\mu^\delta,v^\delta,u^\delta) \in \overline{H}^2_{\partial_n}(\Omega)^M \times \overline{H}^2_{\partial_n}(\Omega)^M \times H^1_{0,\sigma}(\Omega;\mathbb{R}^N)^{M-1} \times \mathbb{R}_+(U_{ad} - \bar u)$. In order to derive the desired system for (p,r,q) from this variational equation, the adjoint of $g'(\bar\varphi,\bar\mu,\bar v,\bar u)$ has to be calculated.

Exemplarily, we show this calculation for two terms. First, consider the term $\operatorname{div}(v_{i+1} \otimes (\rho'(\varphi_{i-1})\varphi_{i-1}^\delta v_i))$ which gets tested by q_i. Notice that for vector fields $z^{(1)}, z^{(2)}, z^{(3)}$ in $H^1(\Omega;\mathbb{R}^N)$ with $z^{(2)}|_{\partial\Omega} = 0$ we have

$$\int_\Omega z^{(3)} \cdot \operatorname{div}(z^{(2)} \otimes z^{(1)}) = -\int_\Omega z^{(2)} \cdot (Dz^{(3)})z^{(1)}, \quad (4.38)$$

by Gauß' theorem. Hence we get

$$\begin{aligned} \langle \operatorname{div}(v_{i+1} \otimes \rho'(\varphi_{i-1})\varphi_{i-1}^\delta v_i), q_i\rangle &= -\int_\Omega v_{i+1} \cdot (Dq_i)(\rho'(\varphi_{i-1})\varphi_{i-1}^\delta v_i)dx \\ &= -\int_\Omega \rho'(\varphi_{i-1})\varphi_{i-1}^\delta v_i \cdot (Dq_i)^\top v_{i+1}dx. \end{aligned}$$

Secondly, the term $\operatorname{div}(v_{i+1} \otimes -\frac{\rho_2-\rho_1}{2}m(\varphi_{i-1})\nabla\mu_i^\delta)$ gets tested by q_i. This yields

$$\begin{aligned} &\langle \operatorname{div}(v_{i+1} \otimes -\frac{\rho_2-\rho_1}{2}m(\varphi_{i-1})\nabla\mu_i^\delta), q_i\rangle \\ &= \int_\Omega v_{i+1} \cdot (Dq_i)(\frac{\rho_2-\rho_1}{2}m(\varphi_{i-1})\nabla\mu_i^\delta)dx \quad (4.39) \\ &= \int_\Omega \frac{\rho_2-\rho_1}{2}m(\varphi_{i-1})\nabla\mu_i^\delta \cdot (Dq_i)^\top v_{i+1}dx \quad (4.40) \\ &= \int_\Omega \mu_i^\delta \operatorname{div}(-\frac{\rho_2-\rho_1}{2}m(\varphi_{i-1})(Dq_i)^\top v_{i+1})dx \quad (4.41) \end{aligned}$$

since $v_{i+1}|_{\partial\Omega} = 0$. The other terms can be treated similarly. After collecting all terms which contain φ_i^δ, μ_i^δ and v_i^δ, respectively, it follows that

$$
\begin{aligned}
&g'(\bar\varphi,\bar\mu,\bar v,\bar u)^*(p,r,q)\\
&= \left(\begin{array}{l}
\left(\begin{array}{l}
-\frac{1}{\tau}(p_i - p_{i-1}) + a(m'(\varphi_i),\mu_{i+1},p_i) - \operatorname{div}(p_i v_{i+1})\\
\quad -\Delta^t r_{i-1} + \Psi_0^{(k)''}(\varphi_i)^* r_{i-1} - \kappa r_{i+1}\\
\quad -\rho'(\varphi_i)v_{i+1}\cdot\frac{1}{\tau}(q_{i+1}-q_i)\\
\quad -(\rho'(\varphi_i)v_{i+1} - \frac{\rho_2-\rho_1}{2}m'(\varphi_i)\nabla\mu_{i+1})(Dq_{i+1})^\top v_{i+2}\\
\quad +2\eta'(\varphi_i)\varepsilon(v_{i+1}) : Dq_i + \operatorname{div}(\mu_{i+1}q_i)
\end{array}\right)_{i=0}^{M-1}\\
\left(\begin{array}{l}
-r_{i-1} + b(m(\varphi_{i-1}),p_{i-1})\\
\quad -\operatorname{div}(\frac{\rho_2-\rho_1}{2}m(\varphi_{i-1})(Dq_i)^\top v_{i+1}) - q_{i-1}\cdot\nabla\varphi_{i-1}
\end{array}\right)_{i=1}^{M-1}\\
\left(\begin{array}{l}
-\rho(\varphi_{i-1})\frac{1}{\tau}(q_i - q_{i-1}) - \rho(\varphi_{i-1})(Dq_i)^\top v_{i+1}\\
\quad -(Dq_{i-1})(\rho(\varphi_{i-2})v_{i-1} - \frac{\rho_2-\rho_1}{2}m(\varphi_{i-2})\nabla\mu_{i-1})\\
\quad -\operatorname{div}(2\eta(\varphi_{i-1})\varepsilon(q_{i-1})) + p_{i-1}\nabla\varphi_{i-1}
\end{array}\right)_{i=1}^{M-1}\\
\left(\, -q_{i-1}\,\right)_{i=1}^{M-1}
\end{array}\right).
\end{aligned}
$$

Plugging this into (4.37) and using the fact that $(\varphi^\delta,\mu^\delta,v^\delta,u^\delta)$ can be chosen arbitrarily in $\overline{H}^2_{\partial_n}(\Omega)^M \times \overline{H}^2_{\partial_n}(\Omega)^M \times H^1_{0,\sigma}(\Omega;\mathbb{R}^N)^{M-1} \times \mathbb{R}_+(U_{ad}-\bar u)$, we obtain the desired system for (p,r,q). $\square$

The derived optimality system consists of the adjoint equations (4.20)-(4.22) and the optimality condition (4.23). Since the adjoint states p_i, r_i are a priori only contained in $\overline{L}^2(\Omega)$, the system has to be understood in the very weak sense and includes the artificial operators Δ^t, a, b.

However, due to the regularity properties of the objective functional $\mathscr{J}$ the adjoint states p, r possess a higher regularity. This allows us to deduce a more explicit formulation of the adjoint operators corresponding to Δ^t, a, b as seen below.

Lemma 4.1.1. *Suppose that the assumptions of Theorem 4.1.2 are fulfilled. Then* $(p,r) \in \overline{H}^1(\Omega)^M \times \overline{H}^1(\Omega)^{M-1}$ *and it holds that*

$$a(m'(\varphi_i),\mu_{i+1},p_i) = m'(\varphi_i)\nabla\mu_{i+1}\cdot\nabla p_i \qquad \in \overline{H}^1(\Omega)^*, \tag{4.42}$$

$$b(m(\varphi_{i-1}),p_{i-1}) = -\operatorname{div}(m(\varphi_{i-1})\nabla p_{i-1}) \qquad \in \overline{H}^1(\Omega)^*, \tag{4.43}$$

$$-\Delta^t r_{i-1} = -\Delta r_{i-1} \qquad \in \overline{H}^1(\Omega)^*. \tag{4.44}$$

Proof. We prove the claim by backward induction over i. For $i = M-1$ it holds that convergence proof for non-smooth potentials

$$p_{M-1} = r_{M-1} = 0 \in \overline{H}^1(\Omega). \tag{4.45}$$

Now, we take the induction step from i to $i-1$ assuming that $p_i, r_i \in \overline{H}^1(\Omega)$. The higher regularity of p_i, r_i implies that

$$\begin{aligned}
\langle a(m'(\varphi_i), \mu_{i+1}, p_i), \hat{z}\rangle &= -\int_\Omega p_i \operatorname{div}(m'(\varphi_i)\hat{z}\nabla\mu_{i+1})dx \\
&= \int_\Omega m'(\varphi_i)\hat{z}\nabla\mu_{i+1}\cdot\nabla p_i dx \\
&\leq C||m'(\varphi_i)||_{L^\infty}||\nabla\mu_{i+1}||_{L^4}||\nabla p_i||_{L^2}||\hat{z}||_{L^4} \\
&\leq C||m'(\varphi_i)||_{L^\infty}||\mu_{i+1}||_{H^2}||p_i||_{H^1}||\hat{z}||_{H^1},
\end{aligned}$$

for every $\hat{z} \in \overline{H}^2_{\partial_n}(\Omega)$, where we additionally employed the Neumann boundary for the chemical potential. Consequently, $a(m'(\varphi_i), \mu_{i+1}, p_i)$ corresponds to an element of the dual space $\overline{H}^1(\Omega)^*$.

Similarly, equations (4.20), (4.21) and the regularity assumption on p_i, r_i yield that $\Delta^t r_{i-1}$ and $b(m(\varphi_{i-1}), p_{i-1})$ are contained in $\overline{H}^1(\Omega)^*$. By standard regularity arguments one shows that r_{i-1} and p_{i-1} are indeed elements of $\overline{H}^1(\Omega)$ and the desired relations (4.42)-(4.44) follow at once. $\square$

By inserting (4.42),(4.43),(4.44) into the equations (4.20) and (4.21), we can further specify the adjoint system. This will be used throughout the limit analysis in the following subsection.

4.1.2 The limiting stationarity system for the double-obstacle potential

As noted above, the goal of this section is to derive necessary optimality conditions for the optimal control problem related to the double-obstacle potential by studying the system (4.20)-(4.23) for the limit process $k \to \infty$.

For this purpose, it is mandatory to verify the boundedness of the involved quantities in order to pass to the limit along suitable subsequences. While the boundedness of the state variables is guaranteed by Lemma 2.2.4, the next lemma serves as a convenient tool to constrain the corresponding adjoint states independently of the regularization parameter..

Lemma 4.1.2. *Let $\alpha > 0$ be given and M_1 and M_2 be bounded subsets of $\overline{H}^1(\Omega)^*$ and $H^1_{0,\sigma}(\Omega;\mathbb{R}^N)^*$, respectively. Let $\mathscr{M}$ be the set of all tuples*

$$(\hat{p},\hat{r},\hat{q};\hat{A};h_p,h_r,h_q;\hat{c},\hat{u};\hat{m},\hat{\eta},\hat{\rho}) \tag{4.46}$$

such that

$$
\begin{aligned}
(\hat{p},\hat{r},\hat{q}) &\in \overline{H}^1(\Omega)\times\overline{H}^1(\Omega)\times H^1_{0,\sigma}(\Omega;\mathbb{R}^N),\\
\hat{A} &\in \mathscr{L}(\overline{H}^1(\Omega);\overline{H}^1(\Omega)^*) \textit{ be monotone},\\
(h_r,h_p,h_q) &\in M_1\times M_1\times M_2,\\
(\hat{c},\hat{u}) &\in \overline{H}^1(\Omega)\times H^1(\Omega;\mathbb{R}^N),\\
\hat{m},\hat{\eta},\hat{\rho} &\in L^\infty(\Omega) \textit{ with } 1/\alpha\ge\hat{m},\hat{\eta}\ge\alpha \textit{ and } \hat{\rho}\ge 0 \textit{ a.e. on } \Omega,
\end{aligned}
$$

for which the following system is satisfied

$$\frac{1}{\tau}\langle\hat{p},\phi\rangle+(\nabla\hat{r},\nabla\phi)+\langle\hat{A}\hat{r},\phi\rangle=\langle h_r,\phi\rangle, \tag{4.47}$$

$$-\langle\hat{r},\phi\rangle+(\hat{m}\nabla\hat{p},\nabla\phi)-\langle\hat{q}\cdot\nabla\hat{c},\phi\rangle=\langle h_p,\phi\rangle, \tag{4.48}$$

$$\frac{1}{\tau}\langle\hat{\rho}\hat{q},\psi\rangle+(2\hat{\eta}\varepsilon(\hat{q}),\varepsilon(\psi))-\langle(D\hat{q})\hat{u}-\hat{p}\nabla\hat{c},\psi\rangle=\langle h_q,\psi\rangle \tag{4.49}$$

$$\frac{1}{\tau}\int_\Omega\hat{\rho}|\hat{q}|^2-\langle(D\hat{q})\hat{u},\hat{q}\rangle\ge 0. \tag{4.50}$$

for every $\phi\in\overline{H}^1(\Omega)$ *and* $\psi\in H^1_{0,\sigma}(\Omega;\mathbb{R}^N)$.

Then the set $\{(\hat{p},\hat{r},\hat{q}) : (\hat{p},\hat{r},\hat{q};\hat{A};h_p,h_r,h_q;\hat{c},\hat{u};\hat{m},\hat{\eta},\hat{\rho})\in\mathscr{M}\}$ *is bounded in* $\overline{H}^1(\Omega)\times\overline{H}^1(\Omega)\times H^1_{0,\sigma}(\Omega;\mathbb{R}^N)$.

Proof. By testing (4.47)–(4.49) by $\tau\hat{r}$, $\hat{p}$ and $\hat{q}$, respectively, and summing up we obtain

$$
\begin{aligned}
&\tau\langle h_r,\hat{r}\rangle+\langle h_p,\hat{p}\rangle+\langle h_q,\hat{q}\rangle\\
&=\tau\langle\nabla\hat{r},\nabla\hat{r}\rangle+\tau\langle\hat{A}\hat{r},\hat{r}\rangle+\langle\hat{m}\nabla\hat{p},\nabla\hat{p}\rangle\\
&\quad+\frac{1}{\tau}\langle\hat{\rho}\hat{q},\hat{q}\rangle-\langle(D\hat{q})\hat{u},\hat{q}\rangle+(2\hat{\eta}\varepsilon(\hat{q}),\varepsilon(\hat{q}))\\
&\ge\tau||\hat{r}||^2_{\overline{H}^1(\Omega)}+C\Big(||\hat{p}||^2_{\overline{H}^1(\Omega)}+||\hat{q}||^2_{H^1_{0,\sigma}(\Omega;\mathbb{R}^N)}\Big)
\end{aligned}
$$

for a positive constant C depending only on α and on the constants in Korn's and Poincaré's inequalities. This estimate yields the assertion. □

With the help of Lemma 4.1.2 we finally pass to the limit of the adjoint equations (4.20)-(4.22) and the optimality condition (4.23). For this purpose, we impose two additional conditions on the derivative of $\mathscr{J}$. As discussed in Section 3.3, the resulting system (4.55) corresponds to the stationarity system (3.31) for the reformulated MPCC (3.27).

Theorem 4.1.3 (Stationarity conditions)**.** *Suppose that the following assumptions are satisfied.*

(I) $\mathscr{J}'$ *is a bounded mapping from* $\overline{H}^1(\Omega)^M \times \overline{H}^1(\Omega)^M \times H^1_{0,\sigma}(\Omega;\mathbb{R}^N)^{M-1} \times U_{ad}$ *into* $(\overline{H}^1(\Omega)^M \times \overline{H}^1(\Omega)^M \times H^1_{0,\sigma}(\Omega;\mathbb{R}^N)^{M-1} \times L^2(\Omega;\mathbb{R}^N)^{M-1})^*$.

(II) $\frac{\partial \mathscr{J}}{\partial u}$ *is weakly lower-semicontinuous, i.e. for every weakly convergent sequence*

$$\hat{z}^{(n)} = (\hat{\varphi}^{(n)}, \hat{\mu}^{(n)}, \hat{v}^{(n)}, \hat{u}^{(n)}) \rightharpoonup (\hat{\varphi}, \hat{\mu}, \hat{v}, \hat{u}) = \hat{z} \tag{4.51}$$

in $\overline{H}^2_{\partial_n}(\Omega)^M \times \overline{H}^2_{\partial_n}(\Omega)^M \times H^1_{0,\sigma}(\Omega;\mathbb{R}^N)^{M-1} \times U_{ad}$ *it holds that*

$$\liminf_{n\to\infty} \Big\langle \frac{\partial \mathscr{J}}{\partial u}(\hat{z}^{(n)}), \hat{u}^{(n)} \Big\rangle \geq \Big\langle \frac{\partial \mathscr{J}}{\partial u}(\hat{z}), \hat{u} \Big\rangle. \tag{4.52}$$

For every $n \in \mathbb{N}$ *let*

$$(\varphi^{(n)}, \mu^{(n)}, v^{(n)}, u^{(n)}) \in \overline{H}^2_{\partial_n}(\Omega)^M \times \overline{H}^2_{\partial_n}(\Omega)^M \times H^1_{0,\sigma}(\Omega;\mathbb{R}^N)^{M-1} \times U_{ad}$$

be a minimizer for the nonlinear auxiliary program ($P_{\Psi^{(n)}}$) *and let the triple*

$$(p^{(n)}, r^{(n)}, q^{(n)}) \in \overline{H}^1(\Omega)^M \times \overline{H}^1(\Omega)^M \times H^1_{0,\sigma}(\Omega;\mathbb{R}^N)^{M-1} \tag{4.53}$$

denote the associated adjoint state from Theorem 4.1.2 and Lemma 4.1.1.

Then there exists an element $(\varphi, \mu, v, u, p, r, q)$ *and a subsequence denoted by* $\Big\{(\varphi^{(m)}, \mu^{(m)}, v^{(m)}, u^{(m)}, p^{(m)}, r^{(m)}, q^{(m)})\Big\}_{m\in\mathbb{N}}$ *such that*

$$\varphi^{(m)} \rightharpoonup \varphi \text{ in } \overline{H}^2_{\partial_n}(\Omega)^M, \quad \mu^{(m)} \rightharpoonup \mu \text{ in } \overline{H}^2_{\partial_n}(\Omega)^{M-1}, \tag{4.54a}$$

$$v^{(m)} \rightharpoonup v \text{ in } H^2(\Omega;\mathbb{R}^N)^{M-1}, \quad u^{(m)} \rightharpoonup u \text{ in } L^2(\Omega;\mathbb{R}^N)^{M-1}, \tag{4.54b}$$

$$p^{(m)} \rightharpoonup p \text{ in } \overline{H}^1(\Omega)^M, \quad r^{(m)} \rightharpoonup r \text{ in } \overline{H}^1(\Omega)^{M-1}, \tag{4.54c}$$

$$q^{(m)} \rightharpoonup q \text{ in } H^1_{0,\sigma}(\Omega;\mathbb{R}^N)^{M-1}, \quad \Psi_0^{(m)''}(\varphi_{i+1}^{(m)})^* r_i^{(n)} \rightharpoonup \lambda_i \text{ in } \overline{H}^1(\Omega)^*, \tag{4.54d}$$

for all $i=-1,...,M-2$, and for $z=(\varphi,\mu,v,u)$ and $\tilde{q}_k := q_{k-1}$ it holds that

$$\begin{aligned}
-\frac{1}{\tau}(p_i-p_{i-1})+m'(\varphi_i)\nabla\mu_{i+1}\cdot p_i-\operatorname{div}(p_i v_{i+1})-\Delta r_{i-1}&\\
+\lambda_{i-1}-\kappa r_{i+1}-\frac{1}{\tau}\rho'(\varphi_i)v_{i+1}\cdot(q_{i+1}-q_i)&\\
-(\rho'(\varphi_i)v_{i+1}-\frac{\rho_2-\rho_1}{2}m'(\varphi_i)\nabla\mu_{i+1})(Dq_{i+1})^\top v_{i+2}&\\
+2\eta'(\varphi_i)\varepsilon(v_{i+1}):Dq_i+\operatorname{div}(\mu_{i+1}q_i) &= \frac{\partial\mathscr{J}}{\partial\varphi_i}(z),
\end{aligned} \tag{4.55a}$$

$$\begin{aligned}
-r_{i-1}-\operatorname{div}(m(\varphi_{i-1})\nabla p_{i-1})-\operatorname{div}(\frac{\rho_2-\rho_1}{2}m(\varphi_{i-1})(Dq_i)^\top v_{i+1})&\\
-q_{i-1}\cdot\nabla\varphi_{i-1} &= \frac{\partial\mathscr{J}}{\partial\mu_i}(z),
\end{aligned} \tag{4.55b}$$

$$\begin{aligned}
-\frac{1}{\tau}\rho(\varphi_{j-1})(q_j-q_{j-1})-\rho(\varphi_{j-1})(Dq_j)^\top v_{j+1}&\\
-(Dq_{j-1})(\rho(\varphi_{j-2})v_{j-1}-\frac{\rho_2-\rho_1}{2}m(\varphi_{j-2})\nabla\mu_{j-1})&\\
-\operatorname{div}(2\eta(\varphi_{j-1})\varepsilon(q_{j-1}))+p_{j-1}\nabla\varphi_{j-1} &= \frac{\partial\mathscr{J}}{\partial v_j}(z),
\end{aligned} \tag{4.55c}$$

$$\frac{\partial\mathscr{J}}{\partial u}(z)-\tilde{q} \in \left[\mathbb{R}_+(U_{ad}-u)\right]^+. \tag{4.55d}$$

Proof. The boundedness of the sequence $\left\{(\varphi^{(n)},\mu^{(n)},v^{(n)},u^{(n)})\right\}_{n\in\mathbb{N}}$ in

$$\overline{H}^2_{\partial_n}(\Omega)^M\times\overline{H}^2_{\partial_n}(\Omega)^M\times H^2_{0,\sigma}(\Omega;\mathbb{R}^N)^{M-1}\times L^2(\Omega;\mathbb{R}^N)^{M-1} \tag{4.56}$$

follows directly from Lemma 2.2.4.

For $i=0,...,M-1$, $j=1,...,M-1$ and $n\in\mathbb{N}$ the adjoint system for $(\mathrm{P}_{\Psi^{(n)}})$ corresponding to (4.20)–(4.23) can be rewritten as

$$\begin{aligned}
\frac{1}{\tau}p^{(n)}_{i-1}-\Delta r^{(n)}_{i-1}+\Psi_0^{(n)''}(\varphi_i^{(n)})^* r^{(n)}_{i-1} &= \Theta^{(n)}_{r,i-1}, \qquad (4.57)\\
-r^{(n)}_{j-1}-\operatorname{div}(m(\varphi^{(n)}_{j-1})\nabla p^{(n)}_{j-1})-q^{(n)}_{j-1}\cdot\nabla\varphi^{(n)}_{j-1} &= \Theta^{(n)}_{p,j-1},\\
\frac{1}{\tau}\rho(\varphi^{(n)}_{j-1})q^{(n)}_{j-1}-\operatorname{div}(2\eta(\varphi^{(n)}_{j-1})\varepsilon(q^{(n)}_{j-1}))+p^{(n)}_{j-1}\nabla\varphi^{(n)}_{j-1}&\\
-(Dq_{j-1})(\rho(\varphi^{(n)}_{j-2})v^{(n)}_{j-1}-\frac{\rho_2-\rho_1}{2}m(\varphi^{(n)}_{j-2})\nabla\mu^{(n)}_{j-1}) &= \Theta^{(n)}_{q,j-1},
\end{aligned}$$

where the functionals $\Theta_r^{(n)}$, $\Theta_p^{(n)}$ and $\Theta_q^{(n)}$ are given by

$$
\begin{aligned}
\Theta_{r,i-1}^{(n)} &= \frac{\partial \mathscr{J}}{\partial \varphi_i}(z^{(n)}) + \frac{1}{\tau} p_i^{(n)} - \Big[m'(\varphi_i^{(n)}) \nabla \mu_{i+1}^{(n)} \cdot p_i^{(n)} - \operatorname{div}(p_i^{(n)} v_{i+1}^{(n)}) \\
&\quad - \kappa r_{i+1}^{(n)} - \frac{1}{\tau} \rho(\varphi_i^{(n)})' v_{i+1}^{(n)} \cdot (q_{i+1}^{(n)} - q_i^{(n)}) \\
&\quad + 2\eta(\varphi_i^{(n)})' \varepsilon(v_{i+1}^{(n)}) : Dq_i^{(n)} + \operatorname{div}(\mu_{i+1}^{(n)} q_i^{(n)}) \\
&\quad - (\rho(\varphi_i^{(n)})' v_{i+1}^{(n)} - \frac{\rho_2 - \rho_1}{2} m'(\varphi_i^{(n)}) \nabla \mu_{i+1}^{(n)})(Dq_{i+1}^{(n)})^\top v_{i+2}^{(n)} \Big], \\
\Theta_{p,i-1}^{(n)} &= \frac{\partial \mathscr{J}}{\partial \mu_i}(z^{(n)}) + \operatorname{div}(\frac{\rho_2 - \rho_1}{2} m(\varphi_{i-1}^{(n)})(Dq_i^{(n)})^\top v_{i+1}^{(n)}), \\
\Theta_{q,i-1}^{(n)} &= \frac{\partial \mathscr{J}}{\partial v_i}(z^{(n)}) + \frac{1}{\tau} \rho(\varphi_{i-1}^{(n)}) q_i^{(n)} - \rho(\varphi_{i-1}^{(n)})(Dq_i^{(n)})^\top v_{i+1}^{(n)}.
\end{aligned}
$$

Here, $z^{(n)}$ denotes the tuple $(\varphi^{(n)}, \mu^{(n)}, v^{(n)}, u^{(n)})$.

Below, we prove the boundedness of

$$
\Big\{ (p^{(n)}, r^{(n)}, q^{(n)}) \Big\}_{n \in \mathbb{N}} \subset \overline{H}^1(\Omega)^M \times \overline{H}^1(\Omega)^M \times H^1_{0,\sigma}(\Omega; \mathbb{R}^N)^{M-1} \tag{4.58}
$$

by backward induction over i. If $i \geq M-1$, then $(p_i^{(n)}, r_i^{(n)}, q_i^{(n)}) = 0$ by convention.

In the induction step assume that for $i \in \{0, \ldots, M-1\}$ and for $j \geq i$ the sequence $\{(p_j^{(n)}, r_j^{(n)}, q_j^{(n)})\}_{n \in \mathbb{N}}$ is bounded in $\overline{H}^1(\Omega) \times \overline{H}^1(\Omega) \times H^1_{0,\sigma}(\Omega; \mathbb{R}^N)$.

In combination with the assumptions on $\mathscr{J}$, this implies that the sequence $\{(\Theta_{p,i-1}^{(n)}, \Theta_{r,i-1}^{(n)}, \Theta_{q,i-1}^{(n)})\}_{n \in \mathbb{N}}$ is bounded in $(\overline{H}^1(\Omega) \times \overline{H}^1(\Omega) \times H^1_{0,\sigma}(\Omega; \mathbb{R}^N))^*$. To see this, we exemplary consider two terms. The term $2\eta(\varphi_i^{(n)})' \varepsilon(v_{i+1}^{(n)}) : Dq_i^{(n)}$ is bounded by

$$
\begin{aligned}
\|2\eta(\varphi_i^{(n)})' \varepsilon(v_{i+1}^{(n)}) : Dq_i^{(n)}\|_{L^{6/5}} &\leq C \|\eta(\varphi_i^{(n)})'\|_{L^\infty} \|\varepsilon(v_{i+1}^{(n)})\|_{L^3} \|Dq_i^{(n)}\|_{L^2} \\
&\leq C \|\eta(\varphi_i^{(n)})'\|_{L^\infty} \|v_{i+1}^{(n)}\|_{H^2} \|q_i^{(n)}\|_{H^1}.
\end{aligned}
$$

Moreover, $-\frac{\rho_2 - \rho_1}{2} m'(\varphi_i^{(n)}) \nabla \mu_{i+1}^{(n)} (Dq_{i+1}^{(n)})^\top v_{i+2}^{(n)}$ can be bounded via the estimate

$$
\begin{aligned}
&\| - \frac{\rho_2 - \rho_1}{2} m'(\varphi_i^{(n)}) \nabla \mu_{i+1}^{(n)} (Dq_{i+1}^{(n)})^\top v_{i+2}^{(n)} \|_{L^{6/5}} \\
&\quad \leq C \| - \frac{\rho_2 - \rho_1}{2} m'(\varphi_i^{(n)}) \|_{L^\infty} \|\nabla \mu_{i+1}^{(n)}\|_{L^6} \|Dq_{i+1}^{(n)}\|_{L^2} \|v_{i+2}^{(n)}\|_{L^6} \\
&\quad \leq C \| - \frac{\rho_2 - \rho_1}{2} m'(\varphi_i^{(n)}) \|_{L^\infty} \|\mu_{i+1}^{(n)}\|_{H^2} \|q_{i+1}^{(n)}\|_{H^1} \|v_{i+2}^{(n)}\|_{H^2}.
\end{aligned}
$$

Consequently, these terms define continuous linear functionals on $\overline{H}^1(\Omega)$, which are bounded independently of n. The other summands can be estimated similarly.

For $i > 0$ we apply Lemma 4.1.2 to the following setting

$$
\begin{aligned}
&(\hat{p},\hat{r},\hat{q};\hat{A};h_p,h_r,h_q;\hat{c},\hat{u};\hat{m},\hat{\eta},\hat{\rho}) \\
&:= (p_{i-1}^{(n)},r_{i-1}^{(n)},q_{i-1}^{(n)};\Psi_0^{(n)''}(\varphi_i^{(n)})^*;\Theta_{p,i-1}^{(n)},\Theta_{r,i-1}^{(n)},\Theta_{q,i-1}^{(n)}; \\
&\quad \varphi_{i-1}^{(n)},\rho(\varphi_{i-2}^{(n)})v_{i-1}^{(n)} - \frac{\rho_2-\rho_1}{2}m(\varphi_{i-2}^{(n)})\nabla\mu_{i-1}^{(n)}; \\
&\quad -\frac{\rho_2-\rho_1}{2}m(\varphi_{i-1}^{(n)}),\eta(\varphi_{i-1}^{(n)}),\rho(\varphi_{i-1}^{(n)})).
\end{aligned}
\tag{4.59}
$$

Note that due to $\mathrm{div} v_{i-1}^{(n)} = 0$, we have

$$
\begin{aligned}
\mathrm{div}\,\hat{u} &= \rho(\varphi_{i-2}^{(n)})' v_{i-1}^{(n)}\cdot\nabla\varphi_{i-1}^{(n)} - \mathrm{div}(\frac{\rho_2-\rho_1}{2}m(\varphi_{i-2}^{(n)})\nabla\mu_{i-1}^{(n)}) &(4.60)\\
&= \frac{\rho_2-\rho_1}{2}\left[v_{i-1}^{(n)}\cdot\nabla\varphi_{i-1}^{(n)} - \mathrm{div}(m(\varphi_{i-2}^{(n)})\nabla\mu_{i-1}^{(n)})\right] &(4.61)\\
&= \frac{1}{\tau}\frac{\rho_2-\rho_1}{2}(\varphi_{i-1}^{(n)}-\varphi_{i-2}^{(n)}) \;=\; -\frac{1}{\tau}(\rho(\varphi_{i-1}^{(n)})-\rho(\varphi_{i-2}^{(n)})). &(4.62)
\end{aligned}
$$

With the help of $\int_\Omega\langle(D\hat{q})\hat{u},\hat{q}\rangle = -\int_\Omega\hat{q}\cdot\mathrm{div}(\hat{q}\otimes\hat{u})$ (cf. (4.38)), equation (2.53) yields

$$
\begin{aligned}
&\frac{1}{\tau}\int_\Omega\hat{\rho}|\hat{q}|^2dx - \langle(D\hat{q})\hat{u},\hat{q}\rangle \\
&= \frac{1}{\tau}\int_\Omega\rho(\varphi_{i-1}^{(n)})|q_{i-1}^{(n)}|^2 - \frac{1}{2}(\rho(\varphi_{i-1}^{(n)})-\rho(\varphi_{i-2}^{(n)}))|q_{i-1}^{(n)}|^2dx &(4.63)\\
&= \frac{1}{2\tau}\int_\Omega(\rho(\varphi_{i-2}^{(n)})+\rho(\varphi_{i-1}^{(n)}))|q_{i-1}^{(n)}|^2dx \;\geq\; 0, &(4.64)
\end{aligned}
$$

due to the non-negativity of $\rho(\varphi_{i-2}^{(n)}) \geq 0$ and $\rho(\varphi_{i-1}^{(n)}) \geq 0$, respectively. Hence Lemma 4.1.2 implies the desired boundedness of (4.58).

Note that the case $i = 0$ requires slight modifications to permit the application of Lemma 4.1.2, since (4.22) is not defined for $i = 0$. For this reason, we set

$$
(\hat{q},h_q,\hat{c},\hat{u},\hat{\eta}) = (0,0,0,0,\eta(\varphi_i^{(n)})).
\tag{4.65}
$$

The remaining quantities are defined as above via (4.59) and the rest of the argumentation stays the same. Summing up, we have shown that the sequence

$$
\left\{(\varphi^{(n)},\mu^{(n)},v^{(n)},u^{(n)},p^{(n)},r^{(n)},q^{(n)})\right\}_{n\in\mathbb{N}}
\tag{4.66}
$$

is bounded in the respective product space. From (4.57) it follows that also $\{(\Psi_0^{(n)''}(\varphi_i^{(n)})^* r_{i-1}^{(n)})\}_{n\in\mathbb{N}}$ remains bounded in $\overline{H}^1(\Omega)^*$.

Employing the usual compact embeddings of Sobolev spaces, we arrive at the existence of a weakly convergent subsequence and a corresponding limit point.

Our next step is to pass to the limit in the the adjoint systems (4.20)–(4.23) for $(\mathrm{P}_{\Psi^{(n)}})$. In this process, the limits for the equations (4.20) and (4.21) are considered in $\overline{H}^1(\Omega)^*$ and the limit for (4.22) in $H^1_{0,\sigma}(\Omega;\mathbb{R}^N)^*$.

In the linear terms we can pass to the limit at once.

For $m'(\varphi_i^{(n)})\nabla\mu_{i+1}^{(n)}\cdot p_i^{(n)}$ we verify that $m'(\varphi_i^{(n)})$ converges strongly in $L^\infty(\Omega)$ to $m'(\varphi_i)$, $\nabla\mu_{i+1}^{(n)}$ strongly in $L^{6-\varepsilon}(\Omega)$ to $\nabla\mu_{i+1}$ and $p_i^{(n)}$ weakly in $L^6(\Omega)$ to p_i. Hence,

$$m'(\varphi_i^{(n)})\nabla\mu_{i+1}^{(n)}\cdot p_i^{(n)} \rightharpoonup m'(\varphi_i)\nabla\mu_{i+1}\cdot p_i \text{ in } \overline{H}^1(\Omega)^*. \tag{4.67}$$

Furthermore, we observe that $\frac{\rho_2-\rho_1}{2}m'(\varphi_i^{(n)})$ and $v_{i+2}^{(n)}$ converge strongly in $L^\infty(\Omega)$ to $\frac{\rho_2-\rho_1}{2}m'(\varphi_i)$ and v_{i+2}, respectively. The sequence $\nabla\mu_{i+1}^{(n)}$ converges strongly in $L^{6-\varepsilon}(\Omega)$ to $\nabla\mu_{i+1}$ and $Dq_i^{(n)}$ weakly in $L^2(\Omega)$ to Dq_i. Thus,

$$\frac{\rho_2-\rho_1}{2}m'(\varphi_i^{(n)})\nabla\mu_{i+1}^{(n)}(Dq_{i+1}^{(n)})^\top v_{i+2}^{(n)} \rightharpoonup \frac{\rho_2-\rho_1}{2}m'(\varphi_i)\nabla\mu_{i+1}(Dq_{i+1})^\top v_{i+2}$$

in $\overline{H}^1(\Omega)^*$.

Next, we point out that $\frac{\rho_2-\rho_1}{2}m(\varphi_{i-1}^{(n)})$ and $v_{i+1}^{(n)}$ converge strongly in $L^\infty(\Omega)$ and $q_i^{(n)}$ converges weakly in $L^6(\Omega)$. As a consequence,

$$\operatorname{div}\Big(\frac{\rho_2-\rho_1}{2}m(\varphi_{i-1}^{(n)})(Dq_i^{(n)})^\top v_{i+1}^{(n)}\Big) \rightharpoonup \operatorname{div}\Big(\frac{\rho_2-\rho_1}{2}m(\varphi_{i-1})(Dq_i)^\top v_{i+1}\Big)$$

in $\overline{H}^1(\Omega)^*$.

Moreover, $\eta(\varphi_{i-1}^{(n)})$ converges strongly in $L^\infty(\Omega)$ and $\varepsilon(q_{i-1}^{(n)})$ converges weakly in $L^2(\Omega)$. Hence,

$$\operatorname{div}(2\eta(\varphi_{i-1}^{(n)})\varepsilon(q_{i-1}^{(n)})) \rightharpoonup \operatorname{div}(2\eta(\varphi_{i-1})\varepsilon(q_{i-1})) \text{ in } H^1_{0,\sigma}(\Omega;\mathbb{R}^N)^*. \tag{4.68}$$

Apart from $\Psi_0^{(n)''}(\varphi_i^{(n)})^* r_{i-1}^{(n)}$, all remaining terms appearing on the left hand sides can be treated similarly.

The assumptions on $\mathscr{J}$ imply that

$$\mathscr{J}'(\varphi^{(n)},\mu^{(n)},v^{(n)},u^{(n)}) \rightharpoonup \mathscr{J}'(\varphi,\mu,v,u) \tag{4.69}$$

in $(\overline{H}^2_{\partial_n}(\Omega)^M \times \overline{H}^2_{\partial_n}(\Omega)^M \times H^1_{0,\sigma}(\Omega;\mathbb{R}^N)^{M-1} \times L^2(\Omega;\mathbb{R}^N)^{M-1})^*$. Consequently, equation (4.20) yields the weak convergence of $\Psi_0''(\varphi_i^{(n)})^* r_{i-1}^{(n)}$ in $\overline{H}^1(\Omega)^*$. The corresponding limit point is denoted by λ_{i-1}. In summary, we arrive at the system (4.55a)–(4.55c).

Since $z^{(n)} := (\varphi^{(n)}, \mu^{(n)}, v^{(n)}, u^{(n)})$ is an optimal solution of $(P_{\Psi^{(n)}})$ and $\frac{\partial \mathscr{J}}{\partial u}$ is weakly lower-semicontinuous, we further deduce for $\tilde{q}_k^{(n)} := q_{k-1}^{(n)}$ and an arbitrary $y \in U_{ad}$ that

$$
\begin{aligned}
\langle \tfrac{\partial \mathscr{J}}{\partial u}(z) - \tilde{q}, y - u\rangle &= \langle \tfrac{\partial \mathscr{J}}{\partial u}(z), y\rangle - \langle \tfrac{\partial \mathscr{J}}{\partial u}(z), u\rangle - \langle \tilde{q}, y-u\rangle && (4.70)\\
&\geq \liminf_{n\to\infty} \Big(\langle \tfrac{\partial \mathscr{J}}{\partial u}(z^{(n)}), y\rangle - \langle \tfrac{\partial \mathscr{J}}{\partial u}(z^{(n)}), u^{(n)}\rangle - \langle \tilde{q}^{(n)}, y - u^{(n)}\rangle \Big) && (4.71)\\
&= \liminf_{n\to\infty} \Big(\tfrac{\partial \mathscr{J}}{\partial u}(z^{(n)}) - \tilde{q}^{(n)}, y - u^{(n)}\rangle \Big) && (4.72)\\
&\geq 0, && (4.73)
\end{aligned}
$$

where we additionally utilized the weak and strong convergence of the involved sequences. This shows (4.55d) and finishes the proof. □

We point out that Theorem 4.1.3 holds also true for arbitrary bounded sequences of stationary points for $(P_{\Psi^{(n)}})$ (not only global solutions). In this context we recall that the sequence $\left\{(\varphi^{(n)}, \mu^{(n)}, v^{(n)}, u^{(n)})\right\}_{n\in\mathbb{N}}$ is bounded, if $\left\{u^{(n)}\right\}_{n\in\mathbb{N}}$ is bounded in $L^2(\Omega;\mathbb{R}^N)^{M-1}$ (e.g., if the set U_{ad} is bounded).

In order to complete the derivation of $\mathscr{E}$-almost C-stationarity conditions, the system (4.55) has to be supplemented by the respective complementarity and sign conditions. This is done at the hand of a specific realization of $\Psi^{(k)}$, which we introduce in Definition 4.1.1 below. For this purpose, γ represents the graph of the subdifferential of the indicator function of $[\psi_1, \psi_2]$, i.e.

$$\gamma := \{(x,y) \in \mathbb{R}^2 : y \in \partial i_{[\psi_1,\psi_2]}(x)\}.$$

Definition 4.1.1. *Let a mollifier $\zeta \in C^1(\mathbb{R})$ with $\operatorname{supp}\zeta \subset [-1,1]$, $\int_{\mathbb{R}} \zeta = 1$ and $0 \leq \zeta \leq 1$ a.e. on $\mathbb{R}$, and a function $\theta : \mathbb{R}^+ \to \mathbb{R}^+$, with $\theta(\alpha) > 0$ and $\frac{\theta(\alpha)}{\alpha} \to 0$ as $\alpha \to 0$, be given. For the Yosida approximation γ_α with parameter $\alpha > 0$ of γ we define*

$$
\begin{aligned}
\zeta_\alpha(s) &:= \frac{1}{\alpha}\zeta\Big(\frac{s}{\alpha}\Big), \;\; \widetilde{\gamma}_\alpha := \gamma_\alpha * \zeta_{\theta(\alpha)}, && (4.74)\\
\psi^{(\alpha)}(s) &:= \int_0^s \widetilde{\gamma}_\alpha(t)\,dt, \;\; \Psi_{0,\alpha}(\varphi) := \int_\Omega \psi^{(\alpha)}(\varphi(x))\,dx, && (4.75)
\end{aligned}
$$

and set $\Psi_0^{(n)} := \Psi_{0,\frac{1}{n}}$.

Remark 4.1.1. *Note that $\Psi_0^{(n)}$ is Fréchet differentiable for every $\varphi \in H^1(\Omega)$, and for every $C \in \mathbb{R}$ there exists a constant $C_1 \in \mathbb{R}$ such that the Fréchet derivative satisfies*

$$\Psi_0^{(n)}(\varphi) < C \Rightarrow \|\varphi\| + \|\Psi_0^{(n)\prime}(\varphi)\| \le C_1. \tag{4.76}$$

Moreover, $\Psi_0^{(n)\prime}$ can be identified with the superposition operator corresponding to $\widetilde{\gamma}_{\alpha_n}$, cf. [117]. Since $\widetilde{\gamma}_{\alpha_n}$ is bounded and $\overline{H}^2_{\partial_n}(\Omega)$ embeds continuously into $L^{2-\delta}(\Omega)$ for arbitrarily small $\delta > 0$, it follows that $\Psi_0^{(n)\prime}$ maps $\overline{H}^2_{\partial_n}(\Omega)$ continuously Frèchet-differentiably into $L^2(\Omega)$, see, e.g., [86].

The subsequent theorem establishes various (complementarity type) conditions for the primal and dual variables of the optimal control problem (P_Ψ) from Theorem 4.1.3, if the regularized potentials are defined by Definition 4.1.1, by performing a careful limit analysis of the corresponding terms with respect to a vanishing Yosida parameter.

Theorem 4.1.4 (Limiting $\mathscr{E}$-almost C-stationarity)**.** *Suppose that the assumptions on $\mathscr{J}$ of Theorem 4.1.3 are satisfied. Let $\Psi_0^{(n)}$, $n \in \mathbb{N}$ be the functionals of Definition 4.1.1, and let the tuples $(\varphi^{(m)}, \mu^{(m)}, v^{(m)}, u^{(m)}, p^{(m)}, r^{(m)}, q^{(m)})$, $(\varphi, \mu, v, u, p, r, q)$ be the corresponding primal and dual variables from Theorem 4.1.3. For $i = 0, \ldots, M$, let $a_i^{(m)}$ and $\lambda_i^{(m)}$ be defined by*

$$a_i^{(m)} := \Psi_0^{(m)\prime}(\varphi_i^{(m)}), \quad \lambda_i^{(m)} := \Psi_0^{(m)\prime\prime}(\varphi_i^{(m)})^* r_{i-1}^{(m)}. \tag{4.77}$$

such that

$$a_i^{(m)} \rightharpoonup a_i \text{ in } \overline{L}^2(\Omega), \quad \lambda_i^{(m)} \rightharpoonup \lambda^i \text{ in } \overline{H}^1(\Omega)^*. \tag{4.78}$$

Then, for any Lipschitz function $\Lambda : \mathbb{R} \to \mathbb{R}$ with $\Lambda(\psi_1) = \Lambda(\psi_2) = 0$, it holds that

$$(a_i, \Lambda(\varphi_i))_{L^2} = 0, \qquad (a_i, r_{i-1})_{L^2} = 0, \tag{4.79}$$

$$\langle \lambda_i, \Lambda(\varphi_i) \rangle = 0, \qquad \liminf (\lambda_i^{(m)}, r_{i-1}^{(m)})_{L^2} \ge 0. \tag{4.80}$$

Moreover, for every $\varepsilon > 0$ there exists a measurable subset $\mathscr{I}^\varepsilon_{\varphi_i}$ of the inactive set $\mathscr{I}_{\varphi_i}$ such that $|\mathscr{I}_{\varphi_i} \setminus \mathscr{I}^\varepsilon_{\varphi_i}| < \varepsilon$ and

$$\langle \lambda_i, v \rangle = 0 \qquad \forall v \in \overline{H}^1(\Omega), \ v|_{\Omega \setminus \mathscr{I}^\varepsilon_{\varphi_i}} = 0. \tag{4.81}$$

Proof. The subdifferential γ satisfies $y\Lambda(x) = 0$ if $(x, y) \in \gamma$. Since $(\varphi_i, a_i) \in \gamma$ a.e. on Ω and $a_i \in L^2(\Omega)$, integration yields the complementarity condition $(a_i, \Lambda(\varphi_i))_{L^2} = 0$.

Now we show that $(\lambda_i, \Lambda(\varphi_i))_{L^2} = 0$. It is well-known that the superposition P_K of the metric projection p_K of $\mathbb{R}$ onto $[\psi_1, \psi_2]$ maps $\overline{H}^1(\Omega)$ continuously into itself. Denoting by L_Λ the Lipschitz constant of Λ, it holds that $|\Lambda(s)| \leq L_\Lambda \min(|s - \psi_1|, |s-\psi_2|)$ for $s \in \mathbb{R}$. Using $|\widetilde{\gamma}_\alpha(s)| \leq \frac{1}{\alpha}$ for all s and $\widetilde{\gamma}_\alpha(s) = 0$ for $\psi_1 + \theta(\alpha) \leq s \leq \psi_2 - \theta(\alpha)$ (cf. [117]) yields

$$
\begin{aligned}
|(\lambda_i^{(m)}, \Lambda(P_K(\varphi_i^{(m)})))_{L^2}|^2 &= |(r_i^{(m)}, \Psi_0^{(m)''}(\varphi_i^{(m)})\Lambda(P_K(\varphi_i^{(m)})))_{L^2}|^2 && (4.82)\\
&\leq ||r_i^{(m)}||_{L^2}^2 \int_\Omega |\widetilde{\gamma}_{\alpha_m}(\varphi_i^{(m)})\Lambda(P_K(\varphi_i^{(m)}))|^2 && (4.83)\\
&\leq \left(|\Omega|\,||r_i^{(m)}||_{L^2} L_\Lambda \frac{\theta(\alpha_m)}{\alpha_m}\right)^2 \;\to\; 0, && (4.84)
\end{aligned}
$$

as $m \to \infty$ and consequently

$$
\begin{aligned}
&\lim(\lambda_i^{(m)}, \Lambda(\varphi_i^{(m)}))_{L^2}\\
&= \lim(\lambda_i^{(m)}, \Lambda(P_K(\varphi_i^{(m)})))_{L^2} + \lim\langle \lambda_i^{(m)}, \Lambda(\varphi_i^{(m)}) - \Lambda(P_K(\varphi_i^{(m)}))\rangle_{\overline{H}^1(\Omega)}\\
&= 0, \qquad (4.85)
\end{aligned}
$$

which implies $\langle \lambda_i, \Lambda(\varphi_i)\rangle = 0$, since $\varphi_i^{(m)}$ converges strongly to $\varphi_i = P_K(\varphi_i)$ in $\overline{H}^1(\Omega)$.

In order to show $(a_i, r_i) = 0$, we define $g_m(s) := \widetilde{\gamma}_{\alpha_m}(s) - \widetilde{\gamma}_{\alpha_m}(s)(s - p_K(s))$. Then it holds that

$$
\begin{aligned}
(a_i^{(m)}, r_{i-1}^{(m)})_{L^2} &= \big(r_{i-1}^{(m)}, \widetilde{\gamma}_{\alpha_m}(\varphi_i^{(m)})\big)_{L^2} && (4.86)\\
&= \big(r_{i-1}^{(m)}, g_m(\varphi_i^{(m)})\big)_{L^2} + \big(\lambda_i^{(m)}, \varphi_i^{(m)} - P_K(\varphi_i^{(m)})\big)_{L^2}. && (4.87)
\end{aligned}
$$

Since $|g_m(s)| = |\widetilde{\gamma}_{\alpha_m}(s) - \widetilde{\gamma}_{\alpha_m}(s)(s - p_K(s))| \leq C\frac{\theta(\alpha_m)}{\alpha_m}$ for m sufficiently large (cf. Lemma 4.2 in [117]), the first term on the right-hand side converges to 0. Moreover, the second term tends to zero because of the strong convergence of $(\varphi_i^{(m)})$ and $(P_K(\varphi_i^{(m)}))$ to φ_i in $\overline{H}^1(\Omega)$.

The property $\liminf(\lambda_i^{(m)}, r_{i-1}^{(m)})_{L^2} \geq 0$ follows directly from the monotonicity of $\Psi_0^{(m)''}(\varphi_i^{(m)})$.

The convergence properties of $\varphi_i^{(m)}$ imply that the subset

$$G := \{x \in \Omega : \varphi_i^{(m)}(x) \to \varphi_i(x) \text{ as } m \to \infty\} \subset \Omega \qquad (4.88)$$

has full measure (i.e. $|G| = |\Omega|$). Therefore, for every $x \in G \cap \mathscr{I}_{\varphi_i}$ we can find $m_0(x) \in \mathbb{N}$ with $\psi_1 + \theta(\alpha_m) < \varphi_i^{(m)}(x) < \psi_2 - \theta(\alpha_m)$ for all $m \geq m_0(x)$. Thus,

$$\lambda_i^{(m)}(x) = \widetilde{\gamma}_{\alpha_m}(\varphi_i^{(m)}(x)) r_i^{(m)}(x) \to 0 \text{ a.e. on } G \cap \mathscr{I}_{\varphi_i} \qquad (4.89)$$

The application of Egorov's theorem ensures that for every $\varepsilon > 0$ there exists a subset $\mathscr{I}_{\varphi_i}^{\varepsilon}$ of $G \cap \mathscr{I}_{\varphi_i}$ with $|\mathscr{I}_{\varphi_i} \setminus \mathscr{I}_{\varphi_i}^{\varepsilon}| < \varepsilon$ such that $\lambda_i^{(m)}$ converges uniformly to zero on $\mathscr{I}_{\varphi_i}^{\varepsilon}$. Hence, we obtain

$$\langle \lambda_i, v \rangle = \lim \langle \lambda_i^{(m)}, v \rangle = 0 \qquad \forall v \in \overline{H}^1(\Omega), \;\; v|_{\Omega \setminus \mathscr{I}_{\varphi_i}^{\varepsilon}} = 0, \tag{4.90}$$

which proves the assertion. $\square$

In combination with the adjoint system from Theorem 4.1.3, the last theorem yields stationarity conditions for the optimal control problem (3.27), which relate to a function space version of limiting $\mathscr{E}$- almost C-stationarity. Here, condition (4.79) reflects the complementarity conditions (3.25b), (3.25c) of the primal system, as well as the fact that r vanishes on the strongly active sets, i.e. 3.32. Whereas the equality condition (3.36) and the sign condition on the product of r and λ, which is distinctive for C-stationarity type systems, are depicted by (4.80).

For the underlying problem class, this is currently the most (and, to the best of our knowledge, only) selective stationarity system available.

4.2 Adaptive finite element method

Our goal for the subsequent sections is to supplement our analytical results with an efficient numerical solver for the optimal control problem (P_Ψ), where the objective functional is of tracking type, i.e. it is given by (3.3) or (3.4), and $U_{ad} = L^2(\Omega;\mathbb{R}^N)$. We benefit from the fact that the specific time-discretization in (2.37) represents a first step towards a numerical investigation/realization of the problem.

As in our analytical investigations, the non-differentiability of the control-to-state operator also complicates the development of numerical solution algorithms for (P_Ψ). However, we postpone the discussion of specifically tailored solution methods for mathematical programs with equilibrium constraints to Section 4.3.

In this section, we are concerned with another mayor challenge which is imposed by repeatedly solving the large-scale nonlinear problems associated with the primal and dual systems from the previous section. In particular, the Navier–Stokes type equations alone are well-known for causing an immense computational expense. Therefore, it is desirable to reduce the numerical effort by choosing a beneficial adaptation procedure for the underlying space mesh. More precisely, we want to refine the discretization locally only in regions with large errors while keeping elements coarse wherever possible, see also Section 1.7.

Such an adaptive mesh refinement strategy is even more favorable, as it allows us to integrate the distinct characteristics of solutions to Cahn–Hilliard type systems. These solutions normally maintain a smooth structure on large parts of the domain, whereas most of the information is concentrated at the small regions corresponding to the transition from the bulk phases to the interfacial layers.

For this reason, we derive an adaptive error estimator for the optimal control problem (P_Ψ), where we additionally incorporate the fact that in most practical applications an accurate estimation of the target quantity, i.e., the objective functional is prioritized. Namely, we follow the dual-weighted residual approach for goal-oriented adaptive finite elements. The approach was first introduced in [22, 23] for unconstrained optimal control problems governed by elliptic differential equations. In these works, the mesh adaptation is driven by weighted residual-based a posteriori error estimates which are derived by global duality arguments and include the error in the state, the adjoint state and the control. Later on, the approach was successfully transferred to optimal control problems with control constraints, see, e.g., [104–106, 185], as well as state constraints, see, e.g., [25, 107], where the latter work considers additional error terms coming from data oscillations. We also mention the articles [57, 91, 92, 100], where reliable a-posteriori error bounds for optimal control problems governed by point wise gradient constraints on the state were derived and an adaptive solution algorithm was presented.

In contrast to PDE-constrained optimal control problems, the literature on goal-oriented mesh adaptivity methods with respect to mathematical programs with equilibrium constraints in function spaces appears rather scarce. However, in [41, 108] the method was successfully applied to the optimal control of elliptic variational inequalities. The presented test examples in these works indicate a good numerical behavior also for MPECs in function spaces.

We point out that most common adaptive refinement concepts for phase field models are based on the idea that the order parameter φ or its derivative take different values on the interfacial layers ($-1 < \varphi < 1$ and $|\nabla\varphi| > 0$) than on the bulk phases ($|\varphi| = 1$ and $\nabla\varphi = 0$), see, e.g., [11,29,130] and [89,103], respectively. In [103], reliable and efficient residual based error estimation is proposed for the Cahn–Hilliard system with a relaxed non-smooth double-obstacle free energy. The error estimation is extended to the simulation of two-phase flow based on model 'H' in [101] and on the model (2.27) in [81]. A-posteriori error estimation for the Cahn–Hilliard systems with non-smooth double-obstacle free energy is also proposed in [20, 21], where the authors present a residual based error estimation and verify the reliability of the derived estimator.

In contrast to these concepts, our approach also acknowledges the contributions of the velocity field v (which is included for residual based methods) and the adjoint variables to the total discretization error. In particular, it consists of dual-weighted primal residuals, primal-weighted dual residuals and additional terms representing the error in the complementarity conditions of the dual system.

In the upcoming subsection, we introduce the underlying discretization scheme of our approach.

4.2.1 Discretization of the problem

Following the so called first optimize, then discretize approach, we subsequently provide a spatial discretization of the stationarity system derived in Section 4.1. More precisely, we discretize the reformulated Cahn–Hilliard–Navier–Stokes system (3.27c)-(3.27g), the adjoint system (3.31), and the complementarity conditions (3.33),(3.36).

For this purpose, let $(\mathscr{T}^i)_{i=0}^{M-1} = (\bigcup_{k=1}^{nt} T_k^i)_{i=0}^{M-1}$ denote a sequence of regular triangulations of Ω, cf. [40, Def. 4.4.13], satisfying $\mathscr{T}^i = \overline{\Omega}$, for $i = 0, \dots, M-1$, and such that the L^2-projection is stable in H^1, cf. [39]. On every triangulation $\mathscr{T}^i$ we consider the finite dimensional spaces V_1^i of piecewise linear and globally continuous finite elements,

$$
\begin{aligned}
V_1^i &:= \{\phi \in C(\mathscr{T}^i) \,|\, \phi|_{T_k^i} \in P^1(T_k^i), k = 1, \dots, nt\} && (4.91)\\
&= \operatorname{span}\{\phi_1^i, \dots, \phi_{N_1^i}^i\} \subset H^1(\Omega), && (4.92)
\end{aligned}
$$

and V_2^i of piecewise quadratic and globally continuous finite elements

$$V_2^i := \{\psi \in C(\mathscr{T}^i)^N \mid \psi|_{\partial\Omega} = 0,\ \psi|_{T_k^i} \in P^2(T_k^i)^N,\ k = 1,\dots,nt\} \tag{4.93}$$
$$= \operatorname{span}\{\psi_1^i,\dots,\psi_{N_1^i}^i\} \subset H_0^1(\Omega)^N, \tag{4.94}$$

respectively. Employing the well-established Taylor-Hood finite elements, we denote the fully discrete counterpart to a solution $(\varphi^i,\mu^i,a^i,v^i)$ of (3.27c)-(3.27g) by$(\varphi_h^i,\mu_h^i,a_h^i,v_h^i) \in V_1^i \times V_1^i \times V_1^i \times V_2^i$. At the hands of the Taylor-Hood ansatz we additionally introduce a pressure variable $\xi_h^i \in V_1^i$ such that the solenoidality condition for the velocity is satisfied in a weak sense. Moreover, we introduce the general control space U and the bounded linear operator $B : U \to L^2(\Omega;\mathbb{R}^N)$. Subsequently, we only assume that U is a Banach space, which includes the case $U := L^2(\Omega;\mathbb{R}^N)$. In our numerical tests, however, we choose a finite dimensional control, since the number of control parameters is usually limited in praxis

In summary, we say that the tuple

$$(\varphi_h^{i+1},\mu_h^{i+1},a_h^{i+1},v_h^{i+1},\xi_h^{i+1}) \in (V_1^{i+1}\times V_1^{i+1}\times V_1^{i+1}\times V_2^{i+1}\times V_1^{i+1})$$

satisfies the discrete variant of (3.27c)-(3.27g) for $i = 0,\dots,M-1$, if it holds for every $\phi \in V_1^{i+1}$ and $\psi \in V_2^{i+1}$ that

$$\left\langle \frac{\varphi_h^{i+1} - \Pi^{i+1}\varphi_h^i}{\tau},\phi \right\rangle + \left\langle v_h^{i+1}\nabla\varphi_h^i,\phi\right\rangle + \left(m(\varphi_h^i)\nabla\mu_h^{i+1},\nabla\phi\right) = 0, \tag{4.95a}$$
$$\left(\nabla\varphi_h^{i+1},\nabla\phi\right) + \left\langle a_h^{i+1},\phi\right\rangle - \left\langle \mu_h^{i+1},\phi\right\rangle - \left\langle \kappa\Pi^{i+1}\varphi_h^i,\phi\right\rangle = 0, \tag{4.95b}$$
$$\begin{aligned}\frac{1}{\tau}\left\langle\rho(\varphi_h^i)v_h^{i+1} - \rho(\varphi_h^{i-1})v_h^i,\psi\right\rangle - \left\langle (\mathrm{v}_h^i\nabla)\psi, v_h^{i+1}\right\rangle \\ + \left(2\eta(\varphi_h^i)D_{sy}(v_h^{i+1}),D_{sy}(\psi)\right) - \left\langle \mu_h^{i+1}\nabla\varphi_h^i,\psi\right\rangle \\ - \left\langle \operatorname{div}\psi,\xi_h^i\right\rangle - (Bu^{i+1},\psi) = 0,\end{aligned} \tag{4.95c}$$
$$-(\operatorname{div} v_h^{i+1},\phi) = 0, \tag{4.95d}$$

with $\mathrm{v}_h^i := \rho(\varphi_h^{i-1})v_h^i - \frac{\rho_2-\rho_1}{2}m(\varphi_h^{i-1})\nabla\mu_h^i$, and the subsequent discrete complementarity conditions for the Cahn–Hilliard problem are satisfied

$$\psi_1 \le \varphi_h^{i+1} \le \psi_2 \tag{4.96a}$$
$$(a_h^{i+1})^+ - (a_h^{i+1})^- = a_h^{i+1}, \tag{4.96b}$$
$$((a_h^{i+1})^+,\phi^+) \ge 0,\ ((a_h^{i+1})^-,\phi^+) \ge 0,\ \forall\phi^+ \in V_{1,+}^{i+1} \tag{4.96c}$$
$$((a_h^{i+1})^+,\varphi_h^{i+1} - \psi_2) = 0,\ ((a_h^{i+1})^-,\varphi_h^{i+1} - \psi_1) = 0. \tag{4.96d}$$

Here, $V_{1,+}^{i+1} := \{\phi \in V_1^{i+1} : \phi \ge 0\}$ and $\Pi^{i+1} : L^2(\Omega) \to V_1^{i+1}$ denotes the orthogonal L^2-projection onto $\{\phi \in V_1^{i+1} \mid |\phi| \le 1\}$. Note that the projection is necessary to derive an energy inequality for the fully discrete system, which is a basic requirement to show the existence of a solution to (4.95a)–(4.96d). As in the semi-discrete case (cf. Section 2.2.1), the proof of the energy estimate involves testing (4.95b) with $\varphi_h^{i+1} - \Pi^{i+1}\varphi_h^i$. Due to the projection, the latter is contained in V_1^{i+1} and therefore a valid test function, cf., e.g., [81].

For the above setting, the pair (V_2^i, V_1^i) is LBB-stable and thus admissible for the numerical realization of (3.27g), see, e.g., [84, 128, 184].

Similar to the discretization of the primal system, we also introduce an adjoint pressure variable $\chi_h^i \in V_1^i$ to express the solenoidality of the adjoint state q. Then the fully discretized adjoint system (3.31) reads as follows.

$$
\begin{aligned}
-\frac{1}{\tau}(\langle(p_h^{i+1}, \Pi^{i+1}\phi\rangle - \langle p_h^i, \phi\rangle) + (m'(\varphi_h^i)\nabla\mu_h^{i+1}\cdot\nabla p_h^{i+1}, \phi)& \\
+\langle p_h^{i+1}v_h^{i+1}, \nabla\phi\rangle + \langle\nabla r_h^i, \nabla\phi\rangle + (\lambda_h^i, \phi) - \langle\kappa r_h^{i+1}, \Pi^{i+1}\phi\rangle& \\
-\left\langle \frac{1}{\tau}\rho'(\varphi_h^i)v_h^{i+1}(q_h^{i+2} - q_h^{i+1}), \phi\right\rangle& \\
-\left\langle \left(\rho(\varphi_h^i)'v_h^{i+1} - \frac{\rho_2-\rho_1}{2}m'(\varphi_h^i)\nabla\mu_h^{i+1}\right)(Dq_h^{i+2})^\top v_h^{i+2}, \phi\right\rangle& \\
+\langle 2\eta(\varphi_h^i)' D_{sy}(v_h^{i+1}) : Dq_h^{i+1}, \phi\rangle& \\
-\langle\mu_h^{i+1}q_h^{i+1}, \nabla\phi\rangle - \left\langle\frac{\partial\mathscr{J}}{\partial\varphi_h^i}(z), \phi\right\rangle &= 0 \quad (4.97a)\\
-\langle r_h^i, \phi\rangle + \langle m(\varphi_h^{i-1})\nabla p_h^i, \nabla\phi\rangle& \\
+\left\langle\frac{\rho_2-\rho_1}{2}m(\varphi_h^{i-1})(Dq_h^{i+1})^\top v_h^{i+1}, \nabla\phi\right\rangle& \\
-(q_h^i\nabla\varphi_h^{i-1}, \phi) - \left\langle\frac{\partial\mathscr{J}}{\partial\mu_h^i}(z), \phi\right\rangle &= 0 \quad (4.97b)\\
-\frac{1}{\tau}\langle\rho(\varphi_h^{i-1})(q_h^{i+1} - q_h^i), \psi\rangle - \left\langle\rho(\varphi_h^{i-1})(Dq_h^{i+1})^\top v_h^{i+1}, \psi\right\rangle& \\
-\left\langle (Dq_h^i)(\rho(\varphi_h^{i-2})v_h^{i-1} - \frac{\rho_2-\rho_1}{2}m(\varphi_h^{i-2})\nabla\mu_h^{i-1}), \psi\right\rangle& \\
+\langle 2\eta(\varphi_h^{i-1})D_{sy}(q_h^i), \nabla\psi\rangle + \langle p_h^i\nabla\varphi_h^{i-1}, \psi\rangle& \\
-\langle\chi_h^i, \operatorname{div}\psi\rangle - \left\langle\frac{\partial\mathscr{J}}{\partial v_h^i}(z), \psi\right\rangle &= 0 \quad (4.97c)\\
-\langle\operatorname{div} q_h^i, \psi\rangle &= 0, \quad (4.97d)\\
\langle B^\star q_h^{i-1}, \tilde{u}\rangle_{U^\star,U} - \left\langle\frac{\partial\mathscr{J}}{\partial u^i}(z), \tilde{u}\right\rangle &= 0, \quad (4.97e)\\
r_h^i - \pi_h^i &= 0, \quad (4.97f)
\end{aligned}
$$

where $\phi \in V_1^i$ and $\psi \in V_2^i$ are arbitrary test functions. In the above system, the prolongation operator Π^{i+1} is applied to the test function $\phi \in V_1^i$ in the adjoint equation.

Moreover, the discretized complementarity conditions are given by

$$((\lambda_h^i)^+, \varphi_h^i - \psi_2) = 0, \quad ((\lambda_h^i)^-, \varphi_h^i - \psi_1) = 0, \tag{4.98a}$$

$$(a_h^i, \pi_h^i) = 0, \tag{4.98b}$$

where $(\lambda_h^i)^+$ and $(\lambda_h^i)^-$ are defined nodewise via

$$(\lambda_h^i)^+(x_j) := \begin{cases} \lambda_h^i & \text{if } \lambda_h^i(x_j) > 0, \\ 0 & \text{else,} \end{cases} \quad (\lambda_h^i)^-(x_j) := \begin{cases} -\lambda_h^i & \text{if } \lambda_h^i(x_j) < 0, \\ 0 & \text{else.} \end{cases} \tag{4.99}$$

for every node x_j of $\mathscr{T}^i$.

This leads us to fully discretized stationarity conditions for the optimal control problem (P_Ψ).

Definition 4.2.1. *Let* $\varphi_h^{-1} = \Pi_{H^1}(\varphi_a)$, $v_h^0 = \Pi_L(v_a)$ *be given, where* Π_{H^1} *denotes the* H^1 *projection onto* $\mathscr{T}^0$*, while* Π_L *denotes the Leray projection ([52]) onto* $\mathscr{T}^0$

.

We say that

$$\begin{aligned}
(\varphi_h^i, \mu_h^i) \in (V_1^i)_{i=0}^{M-1} \times (V_1^i)_{i=0}^{M-1}, (v_h^i, \xi_h^i) \in (V_2^i)_{i=1}^{M-1} \times (V_1^i)_{i=1}^{M-1}, \\
(a_h^i) \in \left(V_1^i\right)_{i=0}^{M-1}, (u^i) \in (U^i)_{i=1}^{M-1}, \\
(p_h^i, r_h^i) \in (V_1^i)_{i=0}^{M-1} \times (V_1^i)_{i=0}^{M-1}, (q_h^i, \chi_h^i) \in (V_2^i)_{i=1}^{M-1} \times (V_1^i)_{i=1}^{M-1}, \\
(\pi_h^i, \lambda_h^i) \in (V_1^i)_{i=0}^{M-1} \times \left(V_1^i\right)_{i=0}^{M-1}
\end{aligned}$$

is a discrete stationary point of (P_Ψ)*, if it satisfies the discretized constraint system* (4.95) *the adjoint system* (4.97) *and the complementarity conditions* (4.98) *for every* $i = 0, .., M-1$.

Note that Definition 4.2.1 does not include a discretization of the sign condition in (4.80), since it provides no benefit for the subsequent derivation of the error estimates. Thus, the system (4.95),(4.97),(4.98) corresponds to a discretization of the weak stationarity conditions for (P_Ψ). We further recall that the notions of $\mathscr{E}$-almost (weak) stationarity, almost (weak) stationarity and (weak) stationarity coincide in finite dimensions.

4.2.2 Goal-oriented error estimator

Utilizing the discretization scheme of the previous section, we now derive the goal-oriented error estimator for (P_Ψ). The resulting estimator can simultaneously handle the error in the phase field variables from the Cahn-Hilliard system, the numerical error in the velocity field attributed mainly to the Navier-Stokes equation, as well as the complementarity errors and the dual quantities connected to the adjoint system through a natural scaling. It measures the difference of the objective function at the continuous solution and a discrete approximation, respectively. For the derivation we consider the modified Lagrangian given by (3.29) and, in particular, the associated saddle-point condition for optimal points. In the sequel, we further assume that discrete solutions exist and are sufficiently close to a continuous solution, which is a standard assumption for the dual-weighted residual method.

In order to simplify the notation, we subsequently collect the primal variables in y (representing the state of the optimal control problem) and the dual variables in Φ (representing the adjoint state), respectively, i.e.

$$y := (\varphi, \mu, a, v), \quad \Phi := (p, r, q). \tag{4.100}$$

Employing the definitions of the MPCC-Lagrangian and weak stationarity, we verify that every $\mathscr{E}$-almost weakly stationary point (y,u) of (P_Ψ) satisfies

$$L(y, u, \Phi, \pi, \lambda^+, \lambda^-) = \mathscr{J}(\varphi, \mu, v, u), \tag{4.101}$$

where $(\Phi, \pi, \lambda^+, \lambda^-)$ denote the corresponding multipliers of the stationarity system. Moreover, for an arbitrarily fixed point $(\pi, \lambda^+, \lambda^-)$, the MPCC-Lagrangian $L(\,\cdot\,, \pi, \lambda^+, \lambda^-)$ is at least three times Fréchet differentiable with respect to (y, u, Φ). This yields the following representation of the objective value at a discrete stationary point of (P_Ψ), which is contained in the product space

$$\mathscr{Y}_h := (V_1^M)^3 \times V_2^{M-1} \times U^{M-1} \times (V_1^M)^2 \times V_2^{M-1} \times (V_1^M)^3. \tag{4.102}$$

Lemma 4.2.1. *Let $(y_h, u_h, \Phi_h, \pi_h, \lambda_h^+, \lambda_h^-) \in \mathscr{Y}_h$ be a discrete stationary point for (P_Ψ). Then for every point $(y, u, \Phi) \in N_{(y_h, u_h, \Phi_h)}$ in a neighborhood of (y_h, u_h, Φ_h) it holds that*

$$\begin{aligned}
&\mathscr{J}(\varphi_h, \mu_h, v_h, u_h) && (4.103)\\
&\qquad = L(y, u, \Phi, \pi_h, \lambda_h^+, \lambda_h^-)\\
&\qquad\quad + \frac{1}{2}\nabla_{(y,u,\Phi)} L(y, u, \Phi, \pi_h, \lambda_h^+, \lambda_h^-)((y_h, u_h, \Phi_h) - (y, u, \Phi))\\
&\qquad\quad + \frac{1}{2}\nabla_{(y,u,\Phi)} L(y_h, u_h, \Phi_h, \pi_h, \lambda_h^+, \lambda_h^-)((y_h, u_h, \Phi_h) - (y, u, \Phi))\\
&\qquad\quad + O\left(\|(y_h, u_h, \Phi_h) - (y, u, \Phi)\|_{\mathscr{Y}_f}^3\right), && (4.104)
\end{aligned}$$

where O denotes the Landau symbol Big-O.

Proof. Since $(y_h, u_h, \Phi_h, \pi_h, \lambda_h^+, \lambda_h^-)$ satisfies the discretized stationarity system from Definition 4.2.1, in particular due to (4.95a)-(4.95c), (4.97d),(4.98a) and (4.98b), it holds that

$$\mathscr{J}(\varphi_h, \mu_h, v_h, u_h) = L(y_h, u_h, \Phi_h, \pi_h, \lambda_h^+, \lambda_h^-). \tag{4.105}$$

Here, we additionally employed the fact that Π^{i+1} is the orthogonal projection onto V_1^{i+1}, i.e., $\langle \Pi^{i+1}\varphi_h^i, p_h^{i+1}\rangle = \langle \varphi_h^i, p_h^{i+1}\rangle$ for all $\varphi_h^i \in L^2(\Omega)$ and $p_h^{i+1} \in V_1^{i+1}$.

Applying Taylor's theorem at $x \in \mathscr{Y}_f$ with respect to $f := L(\,\cdot\,, \pi_h, \lambda_h^+, \lambda_h^-) : \mathscr{Y}_f \to \mathbb{R}$ and ∇f, we derive for all $z \in N_x$ in a sufficiently small neighborhood N_x of x the equations

$$f(z) = f(x) + \nabla f(x)(z-x) + \frac{1}{2}\nabla^2 f(x)(z-x)^2 + O(\|z-x\|_{\mathscr{Y}_f}^3), \tag{4.106}$$
$$\nabla f(z) = \nabla f(x) + \nabla^2 f(x)(z-x) + O\left(\|z-x\|_{\mathscr{Y}_f}^2\right). \tag{4.107}$$

Thus, it holds that

$$\begin{aligned} f(z) &= f(x) + \nabla f(x)(z-x) + \frac{1}{2}(\nabla f(z) - \nabla f(x))(z-x) + O\left(\|z-x\|_{\mathscr{Y}_f}^3\right) \\ &= f(x) + \frac{1}{2}\nabla f(x)(z-x) + \frac{1}{2}\nabla f(z)(z-x) + O(\|z-x\|_{\mathscr{Y}_f}^3). \end{aligned} \tag{4.108}$$

By setting $x := (y, u, \Phi)$ and $z := (y_h, u_h, \Phi_h)$, and keeping in mind that $f = L(\,\cdot\,, \pi_h, \lambda_h^+, \lambda_h^-)$ and therefore, e.g.,

$$\nabla f(x)(x-z) = \nabla_{(y,u,\Phi)} L(y, u, \Phi, \pi_h, \lambda_h^+, \lambda_h^-)((y_h, u_h, \Phi_h) - (y, u, \Phi)),$$

we prove the assertion. $\square$

With the help of Lemma 4.2.1, we establish the following estimate for the discretization error with respect to the objective functional. In this context, the index δ denotes the difference of the discrete and the continuous variables, e.g.

$$(y_\delta, u_\delta, \Phi_\delta) := (y_h, u_h, \Phi_h) - (y, u, \Phi). \tag{4.109}$$

Theorem 4.2.1. *Let $(y_h, u_h, \Phi_h, \pi_h, \lambda_h^+, \lambda_h^-)$ be a discrete stationary point for (P_Ψ) and let $(y, u, \Phi, \pi, \lambda^+, \lambda^-)$ be an $\mathscr{E}$-almost weakly stationary point of the optimal* *control problem (P_Ψ). Then it holds that*

$$
\begin{aligned}
\mathscr{J}(\varphi_h,\mu_h,v_h,u_h)-\mathscr{J}(\varphi,\mu,v,u)=\frac{1}{2}&\left(\sum_{i=0}^{M-1}\left\langle a_h^i,\pi^i\right\rangle-\sum_{i=0}^{M-1}\left\langle a^i,\pi_h^i\right\rangle\right)\\
-\frac{1}{2}&\left(\sum_{i=0}^{M-1}\left\langle(\lambda^i)^+,\varphi_h^i-\psi_2\right\rangle-\sum_{i=0}^{M-1}\left\langle(\lambda_h^i)^+,\varphi^i-\psi_2\right\rangle\right)\\
+\frac{1}{2}&\left(\sum_{i=0}^{M-1}\left\langle(\lambda^i)^-,\varphi_h^i-\psi_1\right\rangle-\sum_{i=0}^{M-1}\left\langle(\lambda_h^i)^-,\varphi^i-\psi_1\right\rangle\right)\\
+\frac{1}{2}\nabla_{(y,u,\Phi)}L(y_h,u_h,\Phi_h,\pi_h,&\lambda_h^+,\lambda_h^-)((y_h,u_h,\Phi_h)-(y,u,\Phi))\\
&+O\left(\|(y_h,u_h,\Phi_h)-(y,u,\Phi)\|_{\mathscr{Y}_f}^3\right).
\end{aligned}
\tag{4.110}
$$

Proof. Since (y,u,Φ) is a stationary point, the gradient of the MPCC-Lagrangian with respect to a direction $(y_\delta,u_\delta,\Phi_\delta)$ reduces to

$$
\begin{aligned}
&\nabla_{(y,u,\Phi)}L[y,u,\Phi,\pi_h,\lambda_h^+,\lambda_h^-](y_\delta,u_\delta,\Phi_\delta)\\
&=\sum_{i=-1}^{M-2}\left\langle a_\delta^{i+1},r^{i+1}\right\rangle-\sum_{i=-1}^{M-2}\left\langle(\lambda^{i+1})^+-(\lambda^{i+1})^-,\varphi_\delta^{i+1}\right\rangle\\
&\quad-\sum_{i=0}^{M-1}\left\langle a_\delta^i,\pi_h^i\right\rangle+\sum_{i=0}^{M-1}\left\langle(\lambda_h^i)^+,\varphi_\delta^i\right\rangle-\sum_{i=0}^{M-1}\left\langle(\lambda_h^i)^-,\varphi_\delta^i\right\rangle \qquad (4.111)\\
&=\sum_{i=0}^{M-1}\left\langle a_\delta^i,\pi^i-\pi_h^i\right\rangle-\sum_{i=0}^{M-1}\left\langle(\lambda^i)^+-(\lambda_h^i)^+,\varphi_\delta^i\right\rangle\\
&\quad+\sum_{i=0}^{M-1}\left\langle(\lambda^i)^--(\lambda_h^i)^-,\varphi_\delta^i\right\rangle, \qquad (4.112)
\end{aligned}
$$

where we used the equations (3.27c)-(3.27g),(3.31),(3.33) and (3.36).

On the other hand, the feasibility of (y,u) implies that

$$
\begin{aligned}
L(y,u,\Phi,\pi_h,\lambda_h^+,\lambda_h^-)=\mathscr{J}(\varphi,\mu,v,u)&-\sum_{i=0}^{M-1}\left\langle a^i,\pi_h^i\right\rangle\\
&+\sum_{i=0}^{M-1}\left\langle(\lambda_h^i)^+,\varphi^i-\psi_2\right\rangle-\sum_{i=0}^{M-1}\left\langle(\lambda_h^i)^-,\varphi^i-\psi_1\right\rangle.
\end{aligned}
\tag{4.113}
$$

Inserting these equations into (4.104) leads to

$$
\begin{aligned}
&\mathscr{J}(\varphi_h,\mu_h,v_h,u_h) && (4.114)\\
&=\mathscr{J}(\varphi,\mu,v,u)-\sum_{i=0}^{M-1}\left\langle a^i,\pi_h^i\right\rangle+\sum_{i=0}^{M-1}\left\langle(\lambda_h^i)^+,\varphi^i-\psi_2\right\rangle\\
&\quad-\sum_{i=0}^{M-1}\left\langle(\lambda_h^i)^-,\varphi^i-\psi_1\right\rangle+\frac{1}{2}\sum_{i=0}^{M-1}\left\langle a_h^i-a^i,\pi^i-\pi_h^i\right\rangle\\
&\quad-\frac{1}{2}\sum_{i=0}^{M-1}\left\langle(\lambda^i)^+-(\lambda_h^i)^+,\varphi_h^i-\varphi^i\right\rangle+\frac{1}{2}\sum_{i=0}^{M-1}\left\langle(\lambda^i)^--(\lambda_h^i)^-,\varphi_h^i-\varphi^i\right\rangle\\
&\quad+\frac{1}{2}\nabla_{(y,u,\Phi)}L(y_h,u_h,\Phi_h,\pi_h,\lambda_h^+,\lambda_h^-)((y_h,u_h,\Phi_h)-(y,u,\Phi))\\
&\quad+O\left(\|(y_h,u_h,\Phi_h)-(y,u,\Phi)\|^3_{\mathscr{Y}_f}\right). && (4.115)
\end{aligned}
$$

An appropriate rearrangement of the terms involving the complementarity conditions (3.33) and (3.36) yields the assertion. □

Since $(y_h,u_h,\Phi_h,\pi_h,\lambda_h^+,\lambda_h^-)$ satisfies the discrete stationarity system and taking into account the orthogonality of the projection Π^{i+1}, it holds that

$$\nabla_{(y,u,\Phi)}L(y_h,u_h,\Phi_h,\pi_h,\lambda_h^+,\lambda_h^-)((y^\alpha,u^\alpha,\Phi^\alpha)-(y_h,u_h,\Phi_h))=0 \quad (4.116)$$

for every point $(y^\alpha,u^\alpha,\Phi^\alpha)\in\mathscr{V}_1^2\times\mathscr{V}_2\times\mathscr{V}_1\times\mathscr{V}_2\times\mathscr{V}_1^2\times\mathscr{V}_2$. Thus, the direction $(y_h,u_h,\Phi_h)-(y,u,\Phi)$ in the respective term of (4.110) can be replaced by any difference $(y^\alpha,u^\alpha,\Phi^\alpha)-(y,u,\Phi)$.

The right-hand side of equation (4.110) assembles the weighted primal and dual residuals, and displays the mismatch in the complementarity between the discretized solution and the original one. More precisely, it involves the following four error estimators for the complementarity mismatch for each time step $i\in\{0,..,M-1\}$

$$\eta_{CM1,i}:=\frac{1}{2}\left\langle a_h^i,\pi^i-\pi_h^i\right\rangle,\ \eta_{CM2,i}:=\frac{1}{2}\left\langle\lambda_h^i,\varphi^i-\varphi_h^i\right\rangle, \quad (4.117)$$

$$\eta_{CM3,i}:=\frac{1}{2}\left\langle a^i,\pi^i-\pi_h^i\right\rangle,\ \eta_{CM4,i}:=\frac{1}{2}\left\langle(\lambda^i),\varphi^i-\varphi_h^i\right\rangle. \quad (4.118)$$

Following the ideas of [108, 154], we employ (2.37b) to reformulate the error estimate $\eta_{CM3,i}$ such that

$$\eta_{CM3,i}=\frac{1}{2}\left(-\nabla\varphi^i,\nabla(\pi^i-\pi_h^i)\right)+\frac{1}{2}\left\langle\mu^i+\kappa\varphi^{i-1},\pi^i-\pi_h^i\right\rangle, \quad (4.119)$$

Similarly, $\eta_{CM4,i}$ is reformulated with the help of the adjoint equation (4.97a) such that the measures a^i and λ^i from the continuous solution are removed from our error estimator, which is convenient for numerical realization.

For every $i = -1, .., M-2$ the dual-weighted primal residuals are given by

$$\eta_{CH1,i+1} := \left\langle \frac{\varphi_h^{i+1} - \varphi_h^i}{\tau}, p_\delta^{i+1} \right\rangle + \left\langle v_h^{i+1} \nabla \varphi_h^i, p_\delta^{i+1} \right\rangle + \left(m(\varphi_h^i) \nabla \mu_h^{i+1}, \nabla p_\delta^{i+1} \right), \tag{4.120}$$

$$\eta_{CH2,i+1} := \left\langle -\Delta \varphi_h^{i+1}, r_\delta^{i+1} \right\rangle + \left\langle a_h^{i+1}, r_\delta^{i+1} \right\rangle - \left\langle \mu_h^{i+1}, r_\delta^{i+1} \right\rangle - \left\langle \kappa \varphi_h^i, r_\delta^{i+1} \right\rangle, \tag{4.121}$$

and

$$\begin{aligned}
\eta_{NS,i+1} :=& \left\langle \frac{\rho(\varphi_h^i) v_h^{i+1} - \rho(\varphi_h^{i-1}) v_h^i}{\tau}, q_\delta^{i+1} \right\rangle_{H^{-1},H_0^1} \\
& - \left(v_h^{i+1} \otimes \rho(\varphi_h^{i-1}) v_h^i, \nabla q_\delta^{i+1} \right) \\
& - \left(v_h^{i+1} \otimes \frac{\rho_2 - \rho_1}{2} m(\varphi_h^{i-1}) \nabla \mu_h^i, \nabla q_\delta^{i+1} \right) \\
& + \left(2\eta(\varphi_h^i) D_{sy}(v_h^{i+1}), D_{sy}(q_\delta^{i+1}) \right) \\
& - \left\langle \mu_h^{i+1} \nabla \varphi_h^i, q_\delta^{i+1} \right\rangle_{H^{-1},H_0^1} - \left\langle B u_h^{i+1}, q_\delta^{i+1} \right\rangle_{H^{-1},H_0^1}.
\end{aligned} \tag{4.122}$$

Since the Navier-Stokes equation is only defined for $i \in \{1, .., M-1\}$ based on the chosen discretization, we set $\eta_{NS,0} := 0$ for the sake of a brief notation.

In order to analyse the primal-weighted dual residual, we point out that every discrete stationary point satisfies

$$\left\langle \frac{\partial \mathscr{J}}{\partial u^i}(\varphi_h, \mu_h, v_h, u_h) - B^\star q_h^i, u_\delta^i \right\rangle = 0. \tag{4.123}$$

If $\mathscr{J}$ is given by (3.3), the partial derivatives are given by

$$\frac{\partial \mathscr{J}}{\partial \mu^i}(\varphi_h, \mu_h, v_h, u_h) = 0, \quad \frac{\partial \mathscr{J}}{\partial v^i}(\varphi_h, \mu_h, v_h, u_h) = 0, \tag{4.124}$$

$$\frac{\partial \mathscr{J}}{\partial \varphi^i}(\varphi_h, \mu_h, v_h, u_h) = \varphi_h^i - \varphi_d^i. \tag{4.125}$$

Then the primal-weighted dual residuals are given by

$$\begin{aligned}\eta_{AD\varphi,i} := \Big[&\varphi_h^i - \varphi_d^i - \frac{1}{\tau}(p_h^{i+1} - p_h^i) + m'(\varphi_h^i)\nabla\mu_h^{i+1}\cdot\nabla p_h^{i+1} \\ &- \operatorname{div}(p_h^{i+1} v_h^{i+1}) - \Delta r_h^i + \lambda_h^i - \kappa r_h^{i+1} - \frac{1}{\tau}\rho'(\varphi_h^i) v_h^{i+1}\cdot(q_h^{i+2} - q_h^{i+1}) \\ &- (\rho'(\varphi_h^i) v_h^{i+1} - \frac{\rho_2-\rho_1}{2} m'(\varphi_h^i)\nabla\mu_h^{i+1})(Dq_h^{i+2})^\top v_h^{i+2} \\ &+ 2\eta'(\varphi_h^i) D_{sy}(v_h^{i+1}) : Dq_h^{i+1} + \operatorname{div}(\mu_h^{i+1} q_h^{i+1})\Big](\varphi_\delta^i),\end{aligned} \tag{4.126}$$

$$\begin{aligned}\eta_{AD\mu,i} := \Big[&-r_h^i - \operatorname{div}(m(\varphi_h^{i-1})\nabla p_h^i) \\ &- \operatorname{div}(\frac{\rho_2-\rho_1}{2} m(\varphi_h^{i-1})(Dq_h^{i+1})^\top v_h^{i+1}) - q_h^i\cdot\nabla\varphi_h^{i-1}\Big](\mu_\delta^i),\end{aligned} \tag{4.127}$$

$$\begin{aligned}\eta_{ADv,i} := \Big[&-\frac{1}{\tau}\rho(\varphi_h^{i-1})(q_h^{i+1} - q_h^i) - \rho(\varphi_h^{i-1})(Dq_h^{i+1})^\top v_h^{i+1} \\ &-(Dq_h^i)(\rho(\varphi_h^{i-2}) v_h^{i-1} - \frac{\rho_2-\rho_1}{2} m(\varphi_h^{i-2})\nabla\mu_h^{i-1}) \\ &- \operatorname{div}(2\eta(\varphi_h^{i-1}) D_{sy}(q_h^i)) + p_h^i \nabla\varphi_h^{i-1}\Big](v_\delta^i),\end{aligned} \tag{4.128}$$

for every $i \in \{0,..,M-1\}$ (with $\eta_{ADv,0} := 0$). With the help of Theorem 4.2.1 and the above definitions, the discretization error with respect to the objective function can be represented as

$$\begin{aligned}\mathscr{J}(\varphi_h,\mu_h,v_h,u_h) - \mathscr{J}(\varphi,\mu,v,u) \\ \approx \sum_{i=0}^{M-1} (&\eta_{CM1,i} + \eta_{CM2,i} + \eta_{CM3,i} + \eta_{CM4,i} + \eta_{CH1,i} \\ &+ \eta_{CH2,i} + \eta_{NS,i} + \eta_{AD\varphi,i} + \eta_{AD\mu,i} + \eta_{ADv,i}) \\ &+ O\left(\|(y_h,u_h,\Phi_h) - (y,u,\Phi)\|_{\mathscr{Y}_f}^3\right)\end{aligned} \tag{4.129}$$

Note that the contribution of the higher order term $O\left(\|(y_h,u_h,\Phi_h) - (y,u,\Phi)\|_{\mathscr{Y}_f}^3\right)$ to the overall error estimator can be neglected, since it is comparatively small. Furthermore, the integral structure of these error terms allows a patchwise evaluation on the underlying mesh, see Section 4.3. Apart from the weights φ_δ^i, μ_δ^i and v_δ^i

and p^i_δ, q^i_δ, r^i_δ, respectively, the primal-dual-weighted error estimators only contain discrete quantities. In order to obtain a fully a-posteriori error estimator the continuous solutions are approximated involving a local higher-order approximation based on the respective discrete variables.

4.3 Numerical solution algorithm

In order to complete the discussion on C-stationarity conditions for the optimal control problem (P_Ψ), we present a numerical solver for the problem, which consolidates the analytical results and the goal-oriented error estimator from the previous sections. We maintain the discretization scheme from Section 4.2.1. The final algorithm is illustrated at the hands of two distinct numerical examples in Subsection 4.3.1.

In accordance with the penalization approach of Section 4.1, the solver calculates an approximate solution of the discrete stationarity system for a given triangulation by repeatedly solving the systems (4.95) and (4.97), where the multipliers a_h^i and λ_h^i are replaced by estimations based on a Moreau-Yosida relaxation of the double-obstacle potential. The respective Moreau–Yosida relaxation is given by

$$\Psi_0^\alpha(\varphi) := \frac{1}{3\alpha}\left(|\max(0,\varphi-1)|^3 + |\min(0,\varphi+1)|^3\right), \tag{4.130}$$

where $\alpha > 0$ is a relaxation parameter. A similar Moreau–Yosida relaxation has been successfully employed in [103]. We point out that it is possible to use a Moreau-Yosida regularization of lower order combined with a semi-smooth Newton method here instead, as, e.g., in [111]. However, since we observe no singularities in our numerical tests and achieve a good approximation of feasibility already for moderate relaxation parameters, we choose the above approach for the ease of implementation.

We obtain the relaxed state equations from (4.95) by substituting $\left\langle a_h^{i+1}, \phi\right\rangle$ with $((\Psi_0^\alpha)'(\varphi_h^{i+1}), \phi)_h$, where $(\cdot,\cdot)_h$ represents the lumped inner product

$$(f,g)_h := \int_\Omega I^i(fg)\,dx, \tag{4.131}$$

and I^i denotes the Lagrangian interpolation on V_1^i. Thus, equation (4.95b) is replaced by

$$\left(\nabla\varphi_h^{i+1}, \nabla\phi\right) + ((\Psi_0^\alpha)'(\varphi_h^{i+1}), \phi)_h - \left\langle \mu_h^{i+1}, \phi\right\rangle - \left\langle \kappa\Pi^{i+1}\varphi_h^i, \phi\right\rangle = 0. \tag{4.132}$$

The corresponding optimal control problem is denoted by $(\mathscr{P}_h^\alpha)$. Note that the existence of feasible points for $(\mathscr{P}_h^\alpha)$ and their boundedness with respect to u_h can be proven, e.g., by transferring the existence proof of Theorem 2.2.1 to the discretized problem. Similarly, (λ_h^i, ϕ) is replaced by the term $((\Psi_0^\alpha)''(\varphi_h^i)r_h^i, \phi)$

such that the modified adjoint system includes the equation

$$
\begin{aligned}
-\frac{1}{\tau}(\langle(p_h^{i+1},\Pi^{i+1}\phi\rangle-\langle p_h^i,\phi\rangle)+(m'(\varphi_h^i)\nabla\mu_h^{i+1}\cdot\nabla p_h^{i+1},\phi)&\\
+\langle p_h^{i+1}v_h^{i+1},\nabla\phi\rangle+\langle\nabla r_h^i,\nabla\phi\rangle+((\Psi_0^\alpha)''(\varphi_h^i)r_h^i,\phi)&\\
-\langle\kappa r_h^{i+1},\Pi^{i+1}\phi\rangle-\left\langle\frac{1}{\tau}\rho'(\varphi_h^i)v_h^{i+1}(q_h^{i+2}-q_h^{i+1}),\phi\right\rangle&\\
-\left\langle\left(\rho(\varphi_h^i)'v_h^{i+1}-\frac{\rho_2-\rho_1}{2}m'(\varphi_h^i)\nabla\mu_h^{i+1}\right)(Dq_h^{i+2})^\top v_h^{i+2},\phi\right\rangle&\\
+\langle 2\eta(\varphi_h^i)'D_{sy}(v_h^{i+1}):Dq_h^{i+1},\phi\rangle&\\
-\langle\mu_h^{i+1}q_h^{i+1},\nabla\phi\rangle-\left\langle\frac{\partial\mathscr{J}}{\partial\varphi_h^i}(z),\phi\right\rangle&=0 \qquad (4.133)
\end{aligned}
$$

instead of (4.97a). Since the resulting system corresponds to the first-order optimality conditions of the discrete optimal control problem $(\mathscr{P}_h^\alpha)$, cf. e.g. Theorem 4.1.2, we compute a suitable solution of the modified system by solving the problem $(\mathscr{P}_h^\alpha)$ via a gradient descent method.

If such a solution is successfully calculated, we decrease α until the complementarity conditions (4.96),(4.98) are sufficiently well fulfilled. In order to evaluate (4.96),(4.98) at the solutions of the modified systems we recover a_h^i and λ_h^i based on the convergence results of the Theorems 4.1.3 and 4.1.4 as finite element functions defined by

$$(a_h^i,\phi)\approx((\Psi_0^\alpha(\varphi_h^i))',\phi)_h, \qquad (4.134a)$$

$$(\lambda_h^i,\phi)\approx((\Psi_0^\alpha(\varphi_h^i))''r_h^i,\phi)_h. \qquad (4.134b)$$

In summary, a discrete stationary point of P_Ψ is calculated via Algorithm 3 below.

In our numerical tests we observe that the complementarity conditions (4.98) are better fulfilled than (4.96d) to at least 3 orders of magnitude. For this reason we subsequently derive an estimate for the dependence of (4.96d) on the relaxation parameter α which forms the foundation of our update procedure for α. More precisely, we approximate the term $((\Psi_0^\alpha(\varphi_h^i))',\varphi_h\pm 1)_h\to 0$ for $\alpha\to 0$.

For this purpose, we suppose that φ_h^i is not both active at the upper and the lower bound on one cell, which can be guaranteed by resolving the interface sufficiently well. I.e., we assume that for every cell $T_k^i\in\mathscr{T}^i$ with $\max(0,\varphi_h^i(x)-1)|>0$ for some $x\in T_k^i$ it holds that

$$\min(0,\varphi_h^i+1)|_{T_k^i}=0. \qquad (4.135)$$

Analogously, if $\min(0,\varphi_h^i(x)+1)<0$ for some $x\in T_k^i$, it follows

$$\max(0,\varphi_h^i(x)-1)|_{T_k^i}=0. \qquad (4.136)$$

Data: Initial data: $\varphi_{-1}, \varphi_0, v_0$;
Choose $u_h := u_0, \alpha := \alpha_0$;
repeat
  repeat
    for $i = 1, \dots, M-1$ **do**
      compute a solution $(\varphi_h^i, \mu_h^i, v_h^i)$ to the relaxed primal system (4.95a),(4.132),(4.95c),(4.95d) for the control u_h^i;
    end
    for $i = M-1, \dots, 1$ **do**
      solve the relaxed dual system (4.133),(4.97b)–(4.97d) for (p_h^i, r_h^i, q_h^i) to obtain a descent direction of the reduced objective functional;
    end
    Compute a new iterate u_h via a standard line search;
  until *the optimality condition* (4.97e) *is approximately satisfied*;
  for $i = 1, \dots, M-1$ **do**
    Compute a_h^i, λ_h^i via (4.134);
  end
  decrease α;
until *the complementarity conditions* (4.96),(4.98) *are sufficiently well fulfilled*;

Algorithm 3: penalizeMPEC

With the help of this assumption we can estimate

$$
\begin{aligned}
|(((\Psi_0^\alpha(\varphi_h^i))', \varphi_h \pm 1)_h| &= |(((\Psi_0^\alpha(\varphi_h^i))', \max(0, \varphi_h^i - 1) + \min(0, \varphi_h^i + 1))_h| \\
&\leq \|I^i((\Psi_0^\alpha(\varphi_h^i))')\|_{L^1(\Omega)} \|\max(0, \varphi_h^i - 1) + \min(0, \varphi_h^i + 1)\|_{L^\infty(\Omega)}. \qquad (4.137)
\end{aligned}
$$

Employing the specific form of Ψ_0^α one can show that there exists a constant $C > 0$ such that

$$
\|I^i((\Psi_0^\alpha(\varphi_h^i))')\|_{L^1(\Omega)} \leq C, \tag{4.138}
$$

for every $\alpha > 0$ and

$$
\|\max(0, \varphi_h^i - 1) + \min(0, \varphi_h^i + 1)\|_{L^\infty(\Omega)} \leq C\alpha^{1/2}, \tag{4.139}
$$

cf. [129]. This leads to

$$
|(((\Psi_0^\alpha(\varphi_h^i))', \varphi_h^i \pm 1)_h| \leq C\alpha^{1/2}. \tag{4.140}
$$

Motivated by the last inequality, we approximate the unknown constant C by $C = \theta\alpha^{-1/2}$, where θ represents the maximum complementarity mismatch for

(4.96d) over all time instances. Then we update the relaxation parameter via

$$\alpha_{new} := \left(\frac{0.9 tol_c}{C} \right)^2, \tag{4.141}$$

where tol_c is the desired tolerance for the complementarity conditions and the factor 0.9 is a guard to really get below the desired tolerance.

Adaptive mesh refinement

As discussed above, we supplement Algorithm 3 with an outer mesh adaptation loop in order to keep the computational effort manageable. In other words, we start with a coarse initial mesh which we repeatedly adapt whenever the discretized stationary system and, in particular, the complementarity conditions (4.96),(4.98) are satisfied sufficiently well.

For this purpose, we calculate error indicators η_T^i for all grids $\mathcal{T}^i$ and for all cells T based on the goal-oriented error estimators from Section 4.2. In this process, we evaluate the derived error estimates individually on each cell of the underlying mesh, e.g.

$$\eta_{CM1,i} = \sum_{T \in \mathcal{T}^i} \eta_{CM1,i}^T = \sum_{T \in \mathcal{T}^i} (a_h^i, \pi^i - \pi_h^i)_{|T}. \tag{4.142}$$

and set

$$(-\Delta \varphi_h^{i+1}, r_\delta^i) := \sum_{T \in \mathcal{T}^{i+1}} \left[(-\Delta \varphi_h^{i+1}, r_\delta^i)_{|T} + \sum_{E \subset T} \frac{1}{2} \left([\nabla \varphi_h^{i+1}]_E, r_\delta^i \right)_{|E} \right], \tag{4.143}$$

compare, e.g., [108]. For a pair of cells T^+, T^- with $T^+ \cap T^- = E$ we define the jump of f across the edge E by

$$[f(x_E)]_E := \left(\lim_{x \to x_E, x \in T^+} f(x) - \lim_{x \to x_E, x \in T^-} f(x) \right) \cdot \nu_{T^+,E}, \tag{4.144}$$

where $\nu_{T^+,E}$ is the unit normal on E pointing into T^+. Note that the definition of $[f]_E$ is independent of the permutation of T^+ and T^-.

Moreover, the continuous solutions are approximated by higher-order finite element approximations of the discrete solution based on the procedure described in [108]. More precisely, for the piecewise linear functions (i.e. $\varphi_h^i, \mu_h^i, p_h^i, r_h^i$) we consider a triangle T and use the nodes of the surrounding three triangles to define six points along with the corresponding values of the finite element function under investigation. Then we evaluate the unique quadratic polynomial that interpolates these six points, and use its restriction to T as quadratic finite element approximation to the continuous solution. If T lies on the boundary of Ω there are less than three surrounding triangles. In this case we create virtual triangles by extending T as a parallelogram outside Ω. Furthermore, we also extend the piecewise linear finite element function linearly on this virtual triangle to obtain six points for the interpolation.

For quadratic finite elements we proceed analogously and evaluate a fourth-order polynomial on the given patch of cells, while for boundary cells we extend the given quadratic function as quadratic polynomial outside Ω. In any case we note that the resulting higher-order approximation is a triangle wise polynomial that is discontinuous across edges.

The overall error indicator η_T^i of a given cell T at the time step i is then defined as

$$\begin{aligned}\eta_T^i =&|\eta_{CM1,i}^T| + |\eta_{CM2,i}^T| + |\eta_{CM3,i}^T| + |\eta_{CM4,i}^T| \\ &+ |\eta_{CH1,i}^T| + |\eta_{CH2,i}^T| + |\eta_{NS,i}^T| \\ &+ |\eta_{AD\varphi,i}^T| + |\eta_{AD\mu,i}^T| + |\eta_{ADv,i}^T|.\end{aligned} \tag{4.145}$$

Note that the individual indicators might be negative, while we require a positive measure for the error, and thus take the absolute values of the final sum.

Comparing the individual error indicators of all the cells $T \in \mathscr{T}^i$ for all time steps i we generate the set $\mathscr{M}_r$ as the set with smallest cardinality such that

$$\sum_{T\in\mathscr{M}_r} \eta_T \geq \theta^r \sum_{i=1}^{M} \sum_{T\in\mathscr{T}^i} \eta_T \tag{4.146}$$

for a given parameter $0 < \theta^r < 1$. This can be done with a greedy marking algorithm. As in [103] we further choose $\theta^c \in (0,1)$ and collect all cells with a comparatively small error indicator in

$$\mathscr{M}_c := \left\{ T \in (\mathscr{T}^i)_{i=1}^M \,|\, \eta_T \leq \frac{\theta^c}{\Xi} \sum_{i=1}^{M} \sum_{T\in\mathscr{T}^i} \eta_T \right\}, \tag{4.147}$$

where $\Xi := \sum_{i=1}^M |\mathscr{T}^i|$. We mark all cells in $\mathscr{M}_r$ for refinement and all cells in $\mathscr{M}_c$ for coarsening. Thus, we use the well-known Dörfler marking procedure, cf. [61]. We stress that we do not perform Dörfler marking on each time instance separately, but, as the representation (4.129) suggests, we perform a marking over all cells in the space-time cylinder. The mesh refinement process is terminated if a desired total number of cells $\Xi_{\max}$ is exceeded. The final algorithm is depicted by Algorithm 4 adaptationLoop.

We point out that our initial grid can not be arbitrarily coarse but has to be locally refined at the interfacial region in order to get a meaningful resolution of the interface. For this reason we apply a homogeneous refinement of the interfacial region of the given initial state such that the interface is resolved by around 12 cells. As a consequence, we also had to introduce the above coarsening strategy.

Data: Initial data: $\varphi_{-1}, \varphi_0, v_0, \Xi_{\max}$
repeat
  compute a discrete stationary point via Algorithm 3 penalizeMPEC;
  calculate the error indicators;
  identify the sets $\mathscr{M}_r, \mathscr{M}_c$ of cells to refine/coarsen;
  adapt $(\mathscr{T}^i)_{i=1}^M$ based on $\mathscr{M}_r$ and $\mathscr{M}_c$;
until $\sum_{i=1}^M |\mathscr{T}^i| < \Xi_{\max}$;

Algorithm 4: adaptationLoop

4.3.1 Numerical results

In this section we illustrate the performance of our algorithmic solver at the hands of two examples, which are specifically designed to illustrate some important properties and capabilities of our approach and the adaptive error estimator.

The solver was implemented in C++ using the finite element toolbox FEniCS [140], the PETSc linear algebra backend [17], and the linear solver MUMPS [13]. For the adaptation of the spatial meshes we employed the toolbox ALBERTA [171], whereas the steepest descent method to solve the finite dimensional problems $(\mathscr{P}_h^\alpha)$ was retrieved from the GNU scientific library [1].

First numerical example

In our first numerical example we consider a circular bubble. Our goal is to prevent the bubble from rising. Moreover, we split it into two bubbles that are deformed to rounded squares, which involves a topological change of the regions associated with the bulk phases.

In more detail, the initial phase field is given by a circle, located at $\hat{o} = (0.5, 0.5)^\top$ with radius $\hat{r} = 0.2329$, i.e.

$$\varphi_0(x) = -1 \cdot \begin{cases} \sin((\|x-\hat{o}\| - \hat{r})/\varepsilon) & \text{if } |\|x-\hat{o}\| - \hat{r}| \leq \varepsilon\frac{\pi}{2}, \\ \operatorname{sign}(\|x-\hat{o}\| - \hat{r}) & \text{else}, \end{cases} \tag{4.148}$$

where the interfacial width corresponds to $\varepsilon = 0.02$. In order to introduce the desired phase field we define

$$\varphi_d[o,r](x) = \begin{cases} \sin((\|((x-o)\|^6 - r)/\varepsilon) & \text{if } |\|(x-o)\| - r|/ \leq \varepsilon\frac{\pi}{2}, \\ \operatorname{sign}(\|(x-o)\|^6 - r) & \text{else,} \end{cases} \tag{4.149}$$

which describes a square with smooth corners around o with radius r. We point out that it is not possible to reproduce sharp corners with a physically reasonable control due to the intrinsic nature of the phase field approach. Then the desired state is given by

$$\varphi_d(x) := \varphi_d[(0.25, 0.50)^\top, 0.15](x) \cdot \varphi_d[(0.75, 0.5)^\top, 0.15](x). \tag{4.150}$$

Note that the radius $\hat{r}$ of φ_0 is chosen in accordance with the mass conservation property of the system, i.e. such that $\int_\Omega \varphi_d\, dx = \int_\Omega \varphi_0\, dx$.

The associated fluid parameters are given by $\rho_1 = 1000$, $\rho_2 = 100$, $\eta_1 = 10$, $\eta_2 = 1$, and $\sigma = 24.5 \cdot \frac{2}{\pi}$ and are taken from a benchmark problem for rising bubble dynamics in [124]. Furthermore, we incorporate a gravitational acceleration $g = 0.981$ in the vertical direction and set $m(\varphi) \equiv \frac{1}{25000}$. The time horizon is set to $T = 1.0$ and the time step size is $\tau = 0.00125$.

We assume that the system can be controlled at the corners of each square. More precisely, we consider the following 16 ansatz functions $f[m_k^{ij}, 0.1, c]$ for $1 \leq k, i, j \leq 2$, and $c \in \{0, 1\}$. Here, the vector field

$$\begin{aligned} &(f[m_k^{ij}, \xi, c](x))^\iota \\ &= \begin{cases} \cos\left(\frac{\pi}{2}\|\xi^{-1}(x - m_k^{ij})\|\right)^2 & \text{if } c \equiv \iota \text{ and } \|\xi^{-1}(x - m_k^{ij})\| \leq 1, \\ 0 & \text{else,} \end{cases} \end{aligned} \tag{4.151}$$

which describes an approximation to the Gaussian with local support around the center

$$m_k^{ij} = (0.5 + (-1)^k 0.25 + (-1)^i 0.13, 0.5 + (-1)^j 0.13)^\top. \tag{4.152}$$

The diagonal matrix ξ represents the width of the Gaussian in the coordinate directions. We identify a scalar value for ξ with ξI, where I denotes the identity matrix. The parameter c is the number of the component in which the vector field f is not zero.

The corresponding operator $B : U \to L^2(\Omega, \mathbb{R}^N)$ with $U = \mathbb{R}^{16}$ is given by

$$Bu := \sum_{c=0}^{1} \sum_{i,j,k=0}^{2} u_{ijkc} f[m_k^{ij}, \xi, c],$$

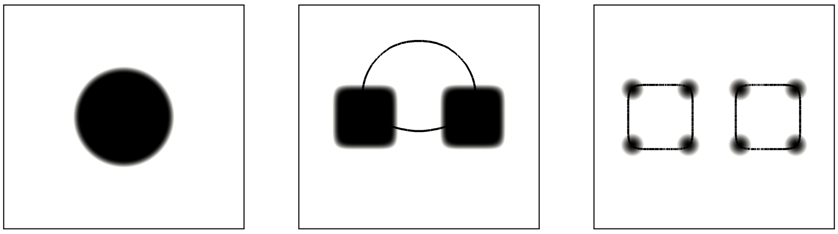

Figure 4.1: The initial shape φ_0, the desired shape φ_d together with the zero level line of the phase field at final time if no control is applied, the ansatz functions for the control together with the zero level line of φ_d (left to right).

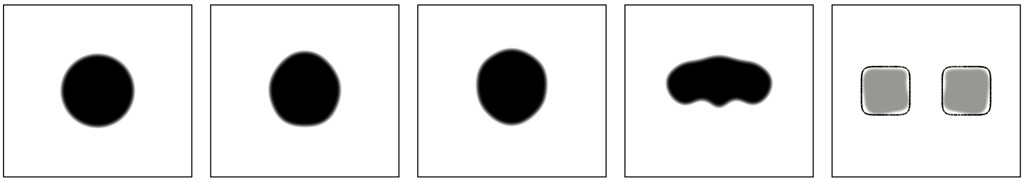

Figure 4.2: The evolution of the phase field φ with respect to the optimal control u for few ansatz functions, $t = 0.00, 0.25, 0.50, 0.75, 1.00$ (left to right). For $t = 1.00$ we show φ in gray and in black the zero level line of the desired shape φ_d.

and we initialize the algorithm with zero control, i.e. $u_0 = 0$.

The plots of φ_0,φ_d, and Bu together with the phase field at final time if no control is applied are depicted in Figure 4.1.

For the marking procedure we use the parameters $\theta^r = 0.7$ and $\theta^c = 0.01$. Furthermore, the stopping criteria use the tolerance $tol_c = 1e-3$ for the complementarity conditions and the maximum amount of cells $\Xi_{max} = 8e6$ for the adaptation process, which relates to $1e4$ cells in average per time instance.

In Figure 4.2 we depict the temporal evolution of the computed optimal phase field $\varphi^\star$ corresponding to the optimal control $u^\star$. Moreover, Figure 4.3 shows the strength of the control over the time horizon, i.e. $|u^\star(t)|$.

The optimal solution on the first level and for the initial value for α was found after 26 steepest descent iterations, while the allover procedure terminated after 419 descent steps.

In our numerical calculations, we observe that the complementarity mismatch appears insensitive with respect to the relaxation parameter α. In other words, once the complementarity mismatch is resolved sufficiently well on the current mesh, α remains unchanged also for the successive grids. In Figure 4.4 we show the evolution of the maximum complementarity mismatch over the optimization steps. Each column of the plot contains the maximum mismatch of the five complementarity relations in (4.96d), (4.98a), and (4.98b), where the maximum is taken over all

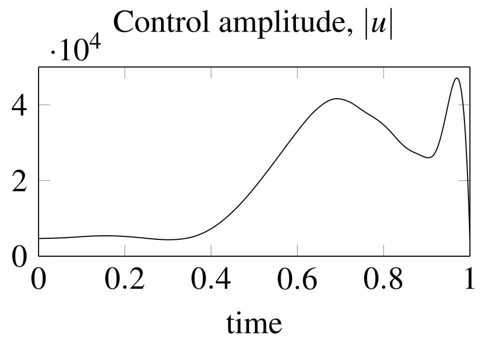

Figure 4.3: The amplitude of the control over time, $|u(t)|$. We observe that the control amplitude is increasing over time until $t = 0.7$ and thereafter is reduced again with a second maximum directly before a final strong reduction of the control at the final time.

time instances and all cells, i.e.

$$ch_p = \max_{i=1,\dots,M} \max_{T \in \mathscr{T}^i} ((a^i)^+, \varphi_h^i - 1)_T, \tag{4.153a}$$

$$ch_m = \max_{i=1,\dots,M} \max_{T \in \mathscr{T}^i} ((a^i)^-, \varphi_h^i + 1)_T, \tag{4.153b}$$

$$ad_p = \max_{i=1,\dots,M} \max_{T \in \mathscr{T}^i} ((\lambda^i)^+, \varphi_h^i - 1)_T, \tag{4.153c}$$

$$ad_m = \max_{i=1,\dots,M} \max_{T \in \mathscr{T}^i} ((\lambda^i)^-, \varphi_h^i + 1)_T, \tag{4.153d}$$

$$api = \max_{i=1,\dots,M} \max_{T \in \mathscr{T}^i} (a^i, \pi^i)_T. \tag{4.153e}$$

The dashed line indicates the desired maximum mismatch tol_c. The algorithm reaches the desired bound after two increments of α. Throughout the subsequent steps α remains unchanged and the algorithm proceeds with the mesh adaptation process directly after the steepest descent method has terminated. The corresponding values of α are $\alpha = 8e6$ as initial value, $\alpha = 3e14$ and finally $\alpha = 6e14$ for subsequent steps. For a rigorous analysis of the error introduced by using the Moreau–Yosida approximation in the case of control of the obstacle-problem we refer to [147].

On the left hand side of Figure 4.5 we present the evolution of the total number of cells over the adaptation steps, whereas the right picture shows the distribution of the cells for the final sequence of grids. Here we illustrate the number of cells of the triangulation $\mathscr{T}^i$ for every time instance and observe a slow increment over time. This can be related to the size of the interfacial region, which also increases with time as the bubble is split up, cf. Figure 4.2.

As expected, the cells are mainly refined inside and, in particular, at the border

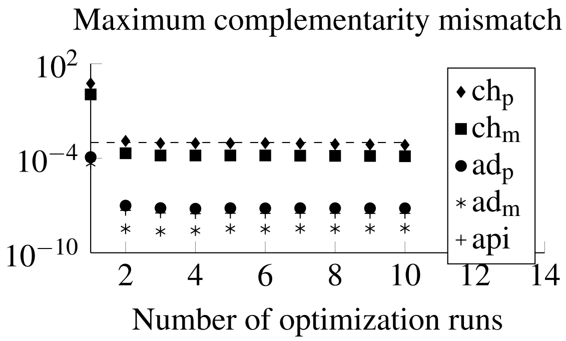

Figure 4.4: The maximum complementarity mismatch for each optimization run, i.e. complete solution of the optimization problem $(\mathscr{P}_h^\alpha)$. Here ch_p, ch_m, ad_p, ad_m and api are defined by (4.153).

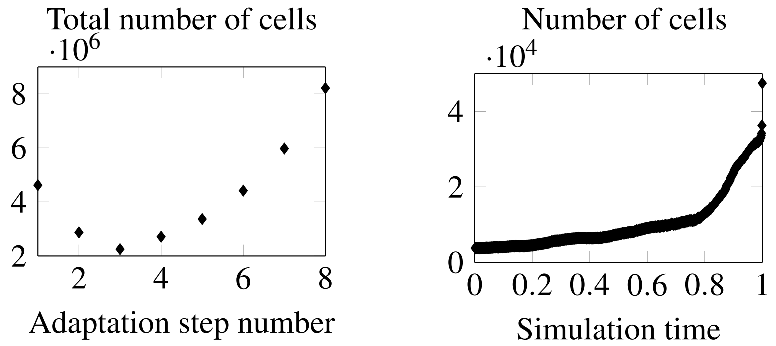

Figure 4.5: The distribution of the total number of cells over the adaptation steps (left) and over the time interval (right).

of the diffuse interface. However, since our dual weighted residual error estimator also contains terms from the Navier–Stokes and the adjoint equation, we further obtain significant mesh adaptations outside of the interface of the phases, which suggests that these errors should not be neglected, e.g. by a simple interface refinement technique. In Figure 4.6 we depict the subdomain $\Omega_u = (0,1)\times(0.5,1.0) \subset \Omega$ at $t = 0.7$. On the left we show $|v|$ in grayscale together with the isolines $\varphi \equiv \pm 1$ in black. On the right we show the corresponding mesh. Note that the mesh is symmetric with respect to the central line.

On the right hand side of Figure 4.7 we portray the evolution of the total estimated error $\eta^i := \sum_{T\in\mathscr{T}^i} \eta_T^i$ at time instance i for the optimal solution $u^\star$. We observe that larger time instances have a higher impact on the overall estimated error. This is a typical behavior for optimal control problems of tracking type which want to push the system towards a desired final state. In particular, the large error at the last time instance can be related to the term $\|\varphi_M - \varphi_d\|$ arising from

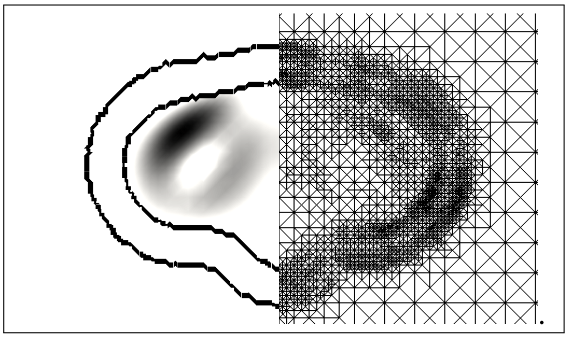

Figure 4.6: The magnitude of v (left) and the corresponding triangulation (right) on the subdomain $(0.0, 1.0) \times (0.25, 0.85) \subset \Omega$ at $t = 0.7$.

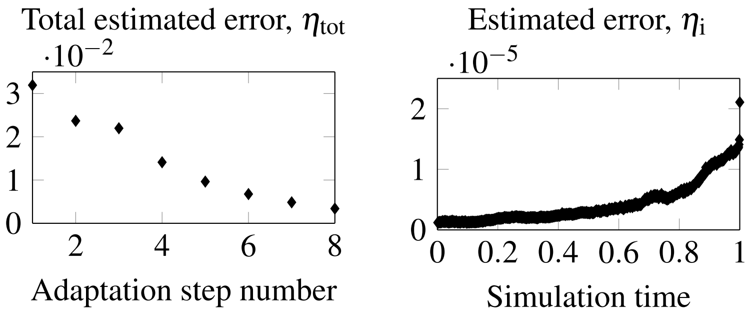

Figure 4.7: The evolution of the error estimator η_{tot} over the adaptation steps (left), the distribution of the estimated error over the time horizon (right).

the optimization aim. Figure 4.7 additionally includes a graph of the total error $\eta_{tot} := \sum_{i=1}^{M} \eta^i$ over all time instances with respect to the adaptation steps, where a significant decay of the estimated error throughout the adaptation steps can be seen.

Second numerical example

In our second example, we aim to form a curved channel out of a ring-shaped initial region. As above, we consider locally supported ansatz functions of the control. These are distributed over the two-dimensional domain as depicted in Figure 4.8.

The quantities $\rho_1, \rho_2, \eta_1, \eta_2, \sigma, g, \tau, T, \theta^r, \theta^c, tol_c, \Xi_{\max}$ are adopted from the first example. Moreover, we set $\varepsilon = 0.04$ and $m(\varphi) \equiv \frac{1}{12500}$.

In Figure 4.9, we present the obtained final state of the algorithm which closely matches the desired state. During the evolution, the ring-shaped initial region is deformed, where the upper part of the ring is pushed towards the top of the domain and the lower part is pushed towards the bottom as it can be seen on the

Figure 4.8: The initial state (left), the desired state (middle) and the control (right) of the optimal control problem.

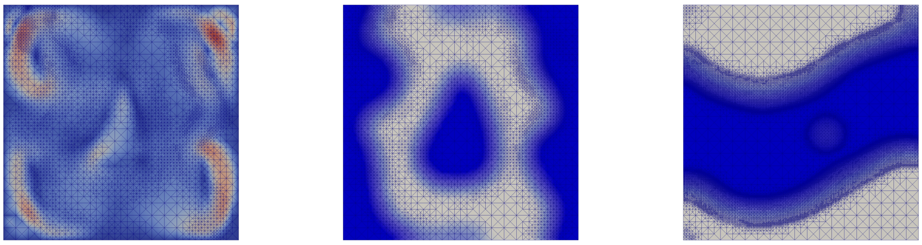

Figure 4.9: The velocity field at time $t = 0.375$ (left), the concentration at $t = 0.375$ (middle) and the obtained final state at $t = 1$ (right).

intermediate state of the process given in Figure 4.9. As a result the phase splits into two separate regions towards the end of the evolution.

The algorithm terminated after 281 gradient steps and 8 adaptation steps, cf. Table 4.1. The decrease of the objective functional is shown in Figure 4.10 with respect to a logarithmic scaling. The small increases in the objective are related to the mesh adaptation, which essentially imposes a different optimization problem in the finite dimensional space.

The right diagram of Figure 4.10 further shows the decrease of the total error estimator as given in (4.129) with respect to the adaptation steps. As it can be

Adaptation step	1			2	3	4
Regularization parameter	1e-07	5e-15	1e-15	1e-15	1e-15	1e-15
Gradient steps	33	111	33	10	14	11
Adaptation step	5	6	7	8	$\sum$	
Regularization parameter	1e-15	1e-15	1e-15	1e-15		
Gradient steps	32	4	22	11	281	

Table 4.1: Number of gradient steps.

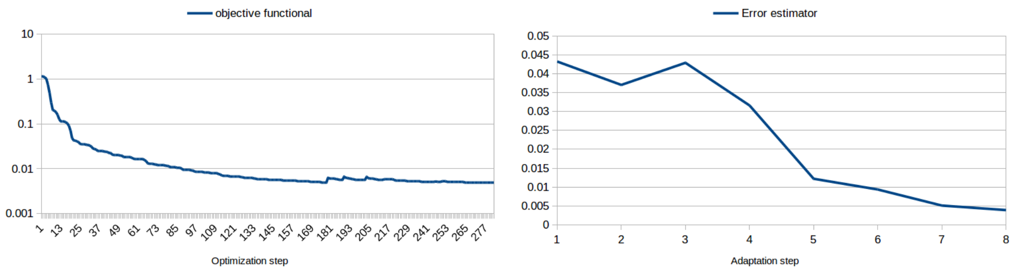

Figure 4.10: The value of the objective functional at each gradient step (left) and the estimated error over all time steps η_{total} at each adaptation step (right).

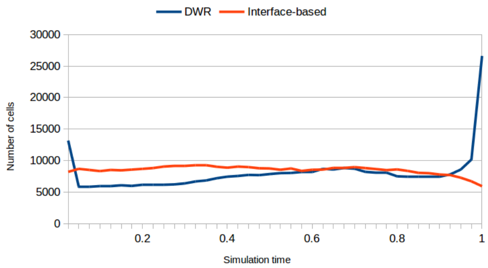

Figure 4.11: The number of cells at each time step for the goal-oriented method and for an adaptation based on the order parameter φ.

seen exemplary in Figure 4.9, the error indicator is dominated by the numerical error connected to the order parameter, which leads to a small resolution of the interfacial boundaries similar to conventional adaptation techniques based on the gradient of φ. Similar to our first example, we additionally observe refinements related to the velocity field outside of the interface, if we compare, e.g., the left and the middle picture of Figure 4.9 which depict the velocity and the order parameter at an intermediate time step along with the corresponding mesh. Furthermore, the goal-oriented error indicator incorporates the structure of the optimization problem which leads to comparatively more refinements at the end of the evolution process. This is illustrated in Figure 4.11, where we compare the distribution of cells over the simulation time for the dual-weighted residuals method and a conventional adaptive method based on φ.

For a comparison of the error decay on a homogeneously refined grid and an adaptively refined grid, where residual based estimation is used for the pure phase field equation, we refer to [103].

Chapter 5

Strong stationarity conditions

5.1 Analytical derivation

In the previous chapter, we derived a C-stationarity system for the optimal control problem (P_Ψ) and successfully implemented a corresponding numerical solution algorithm. Based on these results, it is our goal for this section to establish an even more restrictive stationarity system for (P_Ψ) - namely, strong stationarity.

For this purpose, we verify the Lipschitz continuity of the solution operator of the Cahn–Hilliard–Navier–Stokes system. This allows us to subsequently characterize its directional derivative as the weak limit point of a suitable sequence of the associated difference quotients. A similar idea has been employed for the differentiable sensitivity of an elastic contact problem including a viscous membrane, cf. [127]. From this point on, a technique pioneered by Mignot and Puel in [148, 149], based on a reduction of the optimal control problem by eliminating the state, can be utilized to derive the desired strong stationarity conditions.

Unfortunately, the dependencies of the operators, the corresponding solutions, and their regularity on the interfaces and the previous time steps make this approach very challenging without further restrictive assumptions or additional constraints. For this reason, we choose to pursue a more tractable approach inspired by *finite horizon* model predictive control, see e.g., [79, 121], where a formal discussion and definition can be found. In the context of optimal control of instationary Navier-Stokes this has also been called *instantaneous control problem*, cf. [119, 120].

In this chapter we therefore consider the optimal control of the semi-discrete Cahn–Hilliard–Navier–Stokes system for single time steps. To this end, we assume that the quantities $\varphi_{-1}, \varphi_{-2}, \mu_{-1}, v_{-1}$, which characterize the previous state of the system, are given. In accordance with the observations of Chapter 2, we suppose that the given data has the following regularity

$$(\varphi_{-1}, \varphi_{-2}, \mu_{-1}, v_{-1}) \in \left(H^2_{\partial_n}(\Omega) \cap \mathbb{K}\right)^2 \times H^2_{\partial_n}(\Omega) \times H^2_{0,\sigma}(\Omega;\mathbb{R}^N) \tag{5.1}$$

and satisfies the Cahn–Hilliard equation (2.37a) for the previous time step, i.e.

$$\frac{\varphi_{-1} - \varphi_{-2}}{\tau} + v_{-1}\nabla\varphi_{-2} - \operatorname{div}(m(\varphi_{-1})\nabla\mu_{-1}) = 0. \tag{5.2}$$

For convenience, we briefly recall the resulting Cahn–Hilliard–Navier–Stokes system and the associated optimal control problem. We say that the triple (φ, μ, v) solves the semi-discrete Cahn–Hilliard–Navier–Stokes system for one time step with respect to a given control $u \in H^1_{0,\sigma}(\Omega;\mathbb{R}^N)^*$, if it holds for all $\phi \in H^1(\Omega)$ and

$\psi \in H^1_{0,\sigma}(\Omega;\mathbb{R}^N)$ that

$$\left\langle \frac{\varphi - \varphi_{-1}}{\tau}, \phi \right\rangle + \langle v\nabla\varphi_{-1}, \phi\rangle + (m(\varphi_{-1})\nabla\mu, \nabla\phi) = 0, \tag{5.3a}$$

$$(\nabla\varphi, \nabla\phi) + \langle \partial\Psi_0(\varphi), \phi\rangle - \langle \mu, \phi\rangle - \langle \kappa\varphi_{-1}, \phi\rangle \ni 0, \tag{5.3b}$$

$$\begin{aligned} &\left\langle \frac{\rho(\varphi_{-1})v - \rho(\varphi_{-2})v_{-1}}{\tau}, \psi \right\rangle_{H^{-1}_{0,\sigma}, H^1_{0,\sigma}} - (v \otimes \rho(\varphi_{-2})v_{-1}, \nabla\psi) \\ &+ \left(v \otimes \frac{\rho_2 - \rho_1}{2} m(\varphi_{-2})\nabla\mu_{-1}, \nabla\psi \right) + (2\eta(\varphi_{-1})\varepsilon(v), \varepsilon(\psi)) \\ &\qquad - \langle \mu\nabla\varphi_{-1}, \psi\rangle_{H^{-1}_{0,\sigma}, H^1_{0,\sigma}} = \langle u, \psi\rangle_{H^{-1}_{0,\sigma}, H^1_{0,\sigma}}. \end{aligned} \tag{5.3c}$$

The corresponding solution operator is denoted by

$$\tilde{S}_\Psi : H^1_{0,\sigma}(\Omega;\mathbb{R}^N)^* \to H^1(\Omega) \times H^1(\Omega) \times H^1_{0,\sigma}(\Omega;\mathbb{R}^N), u \to (\varphi, \mu, v). \tag{5.4}$$

Then the optimal control problem under consideration is given as follows.

$$\begin{aligned} &\min \mathscr{J}(\varphi, \mu, v, u) = \frac{1}{2}\|\varphi - \varphi_d\|^2 + \frac{\xi}{2}\|u\|^2 \text{ over } (\varphi, \mu, v, u) \in \tilde{\mathscr{X}} \\ &\text{s.t. } (\varphi, \mu, v) \in \tilde{S}_\Psi(u), \end{aligned} \tag{I_Ψ}$$

where $\varphi_d \in H^1(\Omega), \xi > 0$, and

$$\tilde{\mathscr{X}} := H^1(\Omega) \times H^1(\Omega) \times H^1_{0,\sigma}(\Omega;\mathbb{R}^N) \times L^2(\Omega;\mathbb{R}^N).$$

In contrast to the previous chapters, the mean values of φ and μ are not restricted to zero. In the following, we will briefly show how the results of Chapter 3 and Chapter 4 can be transferred to the current setting.

For the double-well type potentials the existence and regularity of solutions can be deduced analogously to Chapter 2 - Theorem 2.2.1 and Lemma 2.2.2 - with the slight adaptation that it is necessary to employ additional arguments in order to bound the mean values of φ and μ, respectively.

Corollary 5.1.1 (Existence and regularity of solutions)**.** *In the system (5.3) let $\Psi_0^{(k)}$ be given as in Definition 4.1.1 for $k \in \mathbb{N}$ and $u \in H^1_{0,\sigma}(\Omega;\mathbb{R}^N)^*$.*

Then the system (5.3) possesses a solution (φ, μ, v) which is contained in $H^2_{\partial_n}(\Omega) \times H^2_{\partial_n}(\Omega) \times H^1_{0,\sigma}(\Omega;\mathbb{R}^N)$. Furthermore, there exists a constant $C > 0$ depending on $u, N, \Omega, b_1, b_2, \tau, \kappa$ such that

$$\|\varphi\|_{H^2} + \|\mu\|_{H^2} + \|v\|_{H^1} \le C(\|\varphi\| + \|\mu\| + \|\varphi_{-1}\| + \|v\|_{H^1}\|\varphi_{-1}\|_{H^2}). \tag{5.5}$$

If u is contained in $L^2(\Omega;\mathbb{R}^N)$, then $v \in H^2_{0,\sigma}(\Omega;\mathbb{R}^N)$.

Proof. As mentioned above, the first part of the proof is analogous to the proof of Theorem 2.2.1 except for the fact that the operator $\mathscr{G} := (\mathscr{G}_1, \mathscr{G}_2, \mathscr{G}_3)^\top : X \to Y$ is defined on the unrestricted Sobolev spaces

$$
\begin{aligned}
X :=& H^1(\Omega) \times H^1(\Omega) \times H^1_{0,\sigma}(\Omega;\mathbb{R}^N), && (5.6)\\
Y :=& H^1(\Omega)^* \times H^1(\Omega)^* \times H^1_{0,\sigma}(\Omega;\mathbb{R}^N)^*, && (5.7)\\
\overline{Y} :=& L^{\frac{3}{2}}(\Omega) \times L^{\frac{3}{2}}(\Omega) \times L^{\frac{3}{2}}(\Omega;\mathbb{R}^N). && (5.8)
\end{aligned}
$$

via

$$
\begin{aligned}
\langle \mathscr{G}_1(\mu), \phi \rangle &:= (m(\varphi_{-1})\nabla\mu, \nabla\phi) + (\mu, \phi),\\
\langle \mathscr{G}_2(\varphi), \phi \rangle &:= (\nabla\varphi, \nabla\phi) + (\varphi, \phi) + \left\langle \Psi_0^{(k)\prime}(\varphi), \phi \right\rangle,\\
\langle \mathscr{G}_3(v), \psi \rangle_{H^{-1}_{0,\sigma}, H^1_{0,\sigma}} &:= (2\eta(\varphi_{-1})\varepsilon(v), \varepsilon(\psi)) - \langle u, \psi \rangle_{H^{-1}_{0,\sigma}, H^1_{0,\sigma}},
\end{aligned}
$$

and $\mathscr{F} : X \to Y$ is defined accordingly. The compactness of the operator $\mathscr{F} \circ \mathscr{G}^{-1} : \overline{Y} \to \overline{Y}$ follows by the same arguments as before and the existence of a solution δ^* to the fixed point equation

$$
\delta^* - \mathscr{F} \circ \mathscr{G}^{-1}(\delta^*) = 0 \in \overline{Y} \tag{5.9}
$$

is shown with the help of Schaefer's theorem. For this purpose, the boundedness of the set of solutions $(\varphi, \mu, v) \in X$ satisfying the equation

$$
\mathscr{G}(\varphi, \mu, v) - \lambda \mathscr{F}(\varphi, \mu, v) = 0 \tag{5.10}
$$

for an arbitrary $\lambda \in [0,1]$ has to be verified, cf. Subsection 2.2.1. Equation (5.10) is equivalent to the following system of equations

$$
\langle (1-\lambda)\mu, \phi \rangle + \left\langle \lambda \frac{\varphi - \varphi_{-1}}{\tau}, \phi \right\rangle + \langle \lambda v \nabla \varphi_{-1}, \phi \rangle + (m(\varphi_{-1})\nabla\mu, \nabla\phi) = 0, \tag{5.11}
$$

$$
\langle (1-\lambda)\varphi, \phi \rangle + (\nabla\varphi, \nabla\phi) + \left\langle \Psi_0^{(k)\prime}(\varphi)), \phi \right\rangle - \langle \lambda\mu, \phi \rangle - \langle \lambda\kappa\varphi_{-1}, \phi \rangle = 0, \tag{5.12}
$$

$$
\begin{aligned}
&\lambda \left\langle \frac{\rho(\varphi_{-1})v - \rho(\varphi_{-2})v_{-1}}{\tau}, \psi \right\rangle_{H^{-1}_{0,\sigma}, H^1_{0,\sigma}} - \lambda\, (v \otimes \nu, \nabla\psi)\\
&+ (2\eta(\varphi_{-1})\varepsilon(v), \varepsilon(\psi)) - \lambda \,\langle \mu\nabla\varphi_{-1}, \psi \rangle_{H^{-1}_{0,\sigma}, H^1_{0,\sigma}} - \langle u, \psi \rangle_{H^{-1}_{0,\sigma}, H^1_{0,\sigma}} = 0,
\end{aligned} \tag{5.13}
$$

where v is given by

$$v = \rho(\varphi_{-2})v_{-1} - \frac{\rho_2 - \rho_1}{2} m(\varphi_{-2}) \nabla \mu_{-1}. \tag{5.14}$$

Following the same reasoning as in the proof of Theorem 2.2.1, we derive the existence of a constant $C := C(N, \Omega, \tau, \varphi_{-1}, \varphi_{-2}, v_{-1}) > 0$, which is independent of λ, such that

$$\int_\Omega 2\eta(\varphi_{-1}) |\varepsilon(v)|^2 \, dx + \int_\Omega m(\varphi_{-1}) |\nabla \mu|^2 \, dx + \frac{1}{\tau} \Psi^{(k)}(\varphi) + \frac{1}{\tau} \int_\Omega |\nabla \varphi|^2 \, dx \\ + (1-\lambda) \int_\Omega |\mu|^2 dx \leq C + \langle u, v \rangle_{H^{-1}_{0,\sigma}, H^1_{0,\sigma}}. \tag{5.15}$$

Employing Korn's inequality in combination with Assumption 2.1.1.(I), the boundary condition of v, and the lower bound of $\Psi^{(k)}$, we conclude that $\|v\|_{H^1} \leq C_1 := C_1(C, u)$ is bounded.

Moreover, Poincaré's inequality and the boundedness property (4.76) yield the boundedness of $\|\varphi\|_{H^1}$.

It can be further observed that the boundedness of $\|\mu\|_{H^1}$ follows directly from inequality (5.15) if $0 \leq \lambda \leq \frac{1}{2}$ holds true. Otherwise, we conclude that

$$\lambda \int_\Omega \mu dx = (1-\lambda) \int_\Omega \varphi dx - \lambda \kappa \int_\Omega \varphi_{-1} dx + \int_\Omega \Psi_0^{(k)'}(\varphi) dx \tag{5.16}$$

$$\leq C(\|\varphi\| + \|\varphi_{-1}\| + \|\Psi_0^{(k)'}(\varphi)\|) \leq C_1, \tag{5.17}$$

where we used (5.12) and (4.76). In combination with (5.15) and Poincaré's inequality, this ensures $\|\mu\|_{H^1} \leq C$.

The rest of the existence proof and the additional regularity follow analogously to the proofs of Theorem 2.2.1 and Lemma 2.2.2, respectively. $\square$

Now the existence and regularity of solutions to (5.3) for the double-obstacle potential follows at the hands of the convergence theory developed in Section 4.1.

Corollary 5.1.2 (Existence and regularity of solutions)**.** *In the system* (5.3) *let* Ψ_0 *be the double-obstacle potential* $\overline{\Psi}_0$ *given in Assumption 2.1.2. (I) and* $u \in H^1_{0,\sigma}(\Omega; \mathbb{R}^N)^*$. *Then the system* (5.3) *has a solution* $(\varphi, \mu, v) \in H^2_{\partial_n}(\Omega) \times H^2_{\partial_n}(\Omega) \times H^1_{0,\sigma}(\Omega; \mathbb{R}^N)$. *Furthermore, there exists a constant* $C = C(u, N, \Omega, b_1, b_2, \tau, \kappa) > 0$ *such that*

$$\|\varphi\|_{H^2} + \|\mu\|_{H^2} + \|v\|_{H^1} \leq C(\|\varphi\| + \|\mu\| + \|\varphi_{-1}\| + \|v\|_{H^1} \|\varphi_{-1}\|_{H^2}). \tag{5.18}$$

If u *is contained in* $L^2(\Omega; \mathbb{R}^N)$, *then* $v \in H^2_{0,\sigma}(\Omega; \mathbb{R}^N)$.

Proof. Let $\left\{\Psi_0^{(k)}\right\}_{k\in\mathbb{N}}$ be an approximating sequence of double-well type potentials satisfying Definition 4.1.1. Due to Corollary 5.1.1, there exists a bounded sequence $\{(\varphi^{(k)},\mu^{(k)},v^{(k)})\}_{k\in\mathbb{N}} \subset H^2_{\partial_n}(\Omega)\times H^2_{\partial_n}(\Omega)\times H^1_{0,\sigma}(\Omega;\mathbb{R}^N)$ such that the triple $(\varphi^{(k)},\mu^{(k)},v^{(k)})$ solves (5.3) with respect to $\Psi_0^{(k)}$ for every $k\in\mathbb{N}$. Hence there is a weakly convergent subsequence $\left\{(\varphi^{(k_l)},\mu^{(k_l)},v^{(k_l)})\right\}_{l\in\mathbb{N}}$ with the limit point $(\overline{\varphi},\overline{\mu},\overline{v})\in H^2_{\partial_n}(\Omega)\times H^2_{\partial_n}(\Omega)\times H^1_{0,\sigma}(\Omega;\mathbb{R}^N)$.

As in the proof of Theorem 3.2.1 and Theorem 4.1.1, it is shown that the limit point satisfies the system (5.3) with respect to $\overline{\Psi}_0$ and the additional regularity of v is shown analogously to Lemma 2.2.2. □

The existence of globally optimal points of (I_Ψ) can be verified by applying exactly the same arguments as in the proof of Theorem 3.2.1.

Corollary 5.1.3 (Existence of global solutions)**.** *The optimization problem* (I_Ψ) *admits a global solution.*

In the last corollary of this section, we specify the adjoint system for I_Ψ based on Theorem 4.1.3.

Corollary 5.1.4 (Adjoint system)**.** *In the problem* (I_Ψ) *let* $\overline{\Psi}_0$ *be the double-obstacle potential given in Assumption 2.1.2.*

If $\hat{u}$ *is an optimal control of* (I_Ψ)*, then* $\hat{u}\in H^1(\Omega;\mathbb{R}^N)$ *and there exists an adjoint state* $(p,r,s)\in H^1(\Omega)\times H^1(\Omega)\times H^1_{0,\sigma}(\Omega;\mathbb{R}^N)$ *and* $\lambda\in H^1(\Omega)^*$ *such that for all* $\phi\in H^1(\Omega)$ *and* $\psi\in H^1_{0,\sigma}(\Omega;\mathbb{R}^N)$

$$\left\langle D_\varphi \mathscr{J}[\hat{z}]+\frac{r}{\tau},\phi\right\rangle+(\nabla p,\nabla\phi)+\langle\lambda,\phi\rangle=0, \tag{5.19a}$$

$$(m(\varphi_{-1})\nabla r,\nabla\phi)-\langle p,\phi\rangle-\langle s\cdot\nabla\varphi_{-1},\phi\rangle=0, \tag{5.19b}$$

$$\begin{aligned}\left\langle\frac{\rho(\varphi_{-1})}{\tau}s,\psi\right\rangle_{H^{-1}_{0,\sigma},H^1_{0,\sigma}}&-\langle\nabla s v,\psi\rangle_{H^{-1}_{0,\sigma},H^1_{0,\sigma}}\\+(2\eta(\varphi_{-1})\varepsilon(s),\varepsilon(\psi))&-\langle r\nabla\varphi_{-1},\psi\rangle_{H^{-1}_{0,\sigma},H^1_{0,\sigma}}=0\end{aligned} \tag{5.19c}$$

$$\langle -s,\psi\rangle_{H^{-1}_{0,\sigma},H^1_{0,\sigma}}+\langle D_u\mathscr{J}[\hat{z}],\psi\rangle_{H^{-1}_{0,\sigma},H^1_{0,\sigma}}=0, \tag{5.19d}$$

where $\hat{z}:=(\hat{\varphi},\hat{\mu},\hat{v},\hat{u}):=(\tilde{S}_\Psi(\hat{u}),\hat{u})$.

Proof. As above, the same arguments as in the previous chapter (more precisely, as in the proof of Theorem 4.1.3) can be applied. In this process, we additionally need to ensure the boundedness of the corresponding mean values of p, r and s. This is achieved with the help of the following result.

Lemma 5.1.1. *For $k \in \mathbb{N}$ let $\Psi_0^{(k)}$ be given as in Definition 4.1.1. Let $\hat{z}$ be given as in the previous theorem. If $(p,r,s) \in H^1(\Omega) \times H^1(\Omega) \times H^1_{0,\sigma}(\Omega;\mathbb{R}^N)$ satisfies the adjoint system*

$$\left\langle D_\varphi \mathscr{J}[\hat{z}] + \frac{r}{\tau}, \phi \right\rangle + (\nabla p, \nabla \phi) + \left\langle \Psi_0^{(k)''}(\hat{\varphi})^* p, \phi \right\rangle = 0, \tag{5.20a}$$

$$(m(\varphi_{-1})\nabla r, \nabla \phi) - \langle p, \phi \rangle - \langle s \cdot \nabla \varphi_{-1}, \phi \rangle = 0, \tag{5.20b}$$

$$\begin{aligned} &\left\langle \frac{\rho(\varphi_{-1})}{\tau} s, \psi \right\rangle_{H^{-1}_{0,\sigma}, H^1_{0,\sigma}} - \langle \nabla s v, \psi \rangle_{H^{-1}_{0,\sigma}, H^1_{0,\sigma}} \\ &+ (2\eta(\varphi_{-1})\varepsilon(s), \varepsilon(\psi)) - \langle r \nabla \varphi_{-1}, \psi \rangle_{H^{-1}_{0,\sigma}, H^1_{0,\sigma}} = 0, \end{aligned} \tag{5.20c}$$

$$\langle -s, \psi \rangle_{H^{-1}_{0,\sigma}, H^1_{0,\sigma}} + \langle D_u \mathscr{J}[\hat{z}], \psi \rangle_{H^{-1}_{0,\sigma}, H^1_{0,\sigma}} = 0, \tag{5.20d}$$

then the triple $(p,r,s) \in H^1(\Omega) \times H^1(\Omega) \times H^1_{0,\sigma}(\Omega;\mathbb{R}^N)$ is bounded by a constant $C = C(N, \Omega, b_1, b_2, \tau, \hat{\varphi}, \varphi_d) > 0$.

Proof. We test the equations (5.20a)-(5.20c) with τp, r and s, respectively, and sum up to obtain

$$\begin{aligned} \tau \langle D_\varphi \mathscr{J}[\hat{z}], p \rangle + \tau (\nabla p, \nabla p) + \tau \left\langle \Psi_0^{(k)''}(\hat{\varphi})^* p, p \right\rangle + (m(\varphi_{-1})\nabla r, \nabla r) \\ + \left\langle \frac{\rho(\varphi_{-1})}{\tau} s, s \right\rangle_{H^{-1}_{0,\sigma}, H^1_{0,\sigma}} - \langle \nabla s v, s \rangle_{H^{-1}_{0,\sigma}, H^1_{0,\sigma}} \\ + (2\eta(\varphi_{-1})\varepsilon(s), \varepsilon(s)) = 0. \end{aligned} \tag{5.21}$$

As shown in (2.106), it holds that

$$\operatorname{div} v = -\frac{1}{\tau}(\rho(\varphi_{-1}) - \rho(\varphi_{-2})). \tag{5.22}$$

In combination with equation (2.53) and (4.38), this yields

$$\begin{aligned} &\left\langle \frac{\rho(\varphi_{-1})}{\tau} s, s \right\rangle_{H^{-1}_{0,\sigma}, H^1_{0,\sigma}} - \langle \nabla s v, s \rangle_{H^{-1}_{0,\sigma}, H^1_{0,\sigma}} \\ &= \int_\Omega \frac{1}{\tau} \rho(\varphi_{-1}) |s|^2 - \frac{1}{2\tau} (\rho(\varphi_{-1}) - \rho(\varphi_{-2})) |s|^2 dx \qquad (5.23) \\ &= \frac{1}{2\tau} \int_\Omega (\rho(\varphi_{-2}) + \rho(\varphi_{-1})) |s|^2 dx \ \geq \ 0. \qquad (5.24) \end{aligned}$$

By Definition 4.1.1 of the superposition operator $\Psi_0^{(k)}$, it holds that

$$\tau \left\langle \Psi_0^{(k)''}(\hat{\varphi})^* p, p \right\rangle = \tau \int_\Omega \psi^{(\frac{1}{k})''}(\hat{\varphi}) |p|^2 dx \geq 0. \tag{5.25}$$

Further note that $\Psi_0^{(k)''}(\hat{\varphi})^* p$ is an element of $L^2(\Omega)$.

Combining (5.21), (5.24) and (5.25), we infer the existence of a constant $C = C(N, \Omega, b_1, b_2, \tau) > 0$ such that

$$\|\nabla p\|^2 + \|\nabla r\|^2 + \|\varepsilon(s)\|^2 \leq C \left\|D_\varphi \mathscr{J}[\hat{z}]\right\| \|p\|, \tag{5.26}$$

where we also took Assumption 2.1.1.(I) into account.

Since $s \in H^1_{0,\sigma}(\Omega; \mathbb{R}^N)$, testing (5.20b) with $\phi \equiv 1$ yields

$$\int_\Omega p(x) dx = 0. \tag{5.27}$$

Applying Korn's inequality and Poincaré's inequality in combination with the boundary condition for s and (5.27), we obtain

$$\|p\|^2_{H^1} + \|\nabla r\|^2 + \|s\|^2_{H^1} \leq C \left\|D_\varphi \mathscr{J}[\hat{z}]\right\| \|p\|. \tag{5.28}$$

In order to show the boundedness of r in $H^1(\Omega)$ we define $c_r := \frac{1}{|\Omega|} \int_\Omega r(x) dx$ and $w_r := r - c_r$.

Since $\left|\frac{1}{|\Omega|} \int_\Omega \hat{\varphi}(x) dx\right| \neq 1$, there exists a $\delta > 0$ such that $|\Omega_r| := \{|\hat{\varphi}(x)| < 1 - \delta\} > 0$. By definition, the mean value of w_r is equal to zero and we can apply Poincaré's inequality to infer

$$\int_{\Omega_r} w_r dx \leq \int_{\Omega_r} |w_r| dx \leq \|w_r\|_{L^1} \leq C \|\nabla w_r\| = C \|\nabla r\|. \tag{5.29}$$

As all the involved quantities in (5.20a) except for $-\Delta p$ are contained in $L^2(\Omega)$, p is contained in $H^2(\Omega)$, cf. [144, Theorem 2.3.6]. Employing Definition 4.1.1 and equation (5.20a), this yields

$$r = -\tau(\hat{\varphi} - \varphi_d) - \tau \Psi_0^{(k)''}(\hat{\varphi})^* p + \tau \Delta p = -\tau(\hat{\varphi} - \varphi_d) + \tau \Delta p \text{ a.e. on } \Omega_r. \tag{5.30}$$

Hence

$$c_r |\Omega_r| = \int_{\Omega_r} c_r dx = -\tau \int_{\Omega_r} (\hat{\varphi} - \varphi_d) dx + \tau \int_{\Omega_r} \Delta p dx - \int_{\Omega_r} w_r dx \tag{5.31}$$

$$= -\tau \int_{\Omega_r} (\hat{\varphi} - \varphi_d) dx - \tau \int_{\partial \Omega_r} \nabla p \cdot \vec{n} ds - \int_{\Omega_r} w_r dx \tag{5.32}$$

$$\leq C(\|D_\varphi \mathscr{J}[\hat{z}]\| + \|p\|_{H^1} + \|\nabla r\|), \tag{5.33}$$

Thus, the mean value of r is bounded with respect to $\|\nabla r\|$. In combination with Poincaré's inequality and (5.28), this yields the assertion. □

With Lemma 5.1.1 guaranteeing the boundedness of the adjoint state, the adjoint system and the additional regularity of $\hat{u}$ follow from the same arguments as in Theorem 4.1.3. $\square$

An important consequence of the Corollary 5.1.4 is the additional regularity of the optimal control $\hat{u}$ which is employed in Section 5.1.3.

5.1.1 Sensitivity analysis

Throughout the next two sections, we take a closer look at the differentiability and continuity properties of the control-to-state operator $\tilde{S}_{\overline{\Psi}}$. In this section, we start with the Lipschitz continuity of $\tilde{S}_{\overline{\Psi}}$.

For this purpose, and in order to simplify the notation we reformulate the system (5.3) by setting $\mu := \mu + \kappa\varphi_{-1}$ (slightly abusing notation). Then the system can be rewritten as follows

$$\left\langle \frac{\varphi - \varphi_{-1}}{\tau}, \phi \right\rangle + \langle v\nabla\varphi_{-1}, \phi\rangle + (m(\varphi_{-1})\nabla\mu, \nabla\phi) - \kappa(m(\varphi_{-1})\nabla\varphi_{-1}, \nabla\phi) = 0, \tag{5.34a}$$

$$(\nabla\varphi, \nabla\phi) - \langle\mu, \phi\rangle + \langle a, \phi\rangle = 0, \tag{5.34b}$$

$$\begin{aligned}\left\langle \frac{\rho(\varphi_{-1})v - \rho(\varphi_{-2})v_{-1}}{\tau}, \psi \right\rangle_{H^{-1}_{0,\sigma},H^1_{0,\sigma}} &- (v \otimes \rho(\varphi_{-2})v_{-1}, \nabla\psi) \\ + \left(v \otimes \frac{\rho_2 - \rho_1}{2} m(\varphi_{-2})\nabla\mu_{-1}, \nabla\psi \right) &+ (2\eta(\varphi_{-1})\varepsilon(v), \varepsilon(\psi)) \\ - \langle \mu\nabla\varphi_{-1}, \psi\rangle_{H^{-1}_{0,\sigma},H^1_{0,\sigma}} + \langle\kappa\varphi_{-1}\nabla\varphi_{-1}, \psi\rangle_{H^{-1}_{0,\sigma},H^1_{0,\sigma}} &- \langle u, \psi\rangle_{H^{-1}_{0,\sigma},H^1_{0,\sigma}} = 0,\end{aligned} \tag{5.34c}$$

where we additionally used the slack variable $a \in \partial\overline{\Psi}_0(\varphi)$, cf. e.g. Section 3.3.

Clearly, any solution of the system (5.34) can be transformed into a solution of (5.3) by adding/subtracting $\kappa\varphi_{-1}$ to μ and vice versa. For our subsequent investigations we therefore replace the constraint system (5.3) by (5.34) in (I_Ψ) and maintain the same notation.

The subsequent theorem verifies that the solution operator $\tilde{S}_{\overline{\Psi}}$ (to the reformulated system (5.34)) is Lipschitz continuous.

Theorem 5.1.1 (Lipschitz continuity of $\tilde{S}_{\overline{\Psi}}$). *The mapping $\tilde{S}_{\overline{\Psi}} : H^1_{0,\sigma}(\Omega;\mathbb{R}^N)^* \to H^1(\Omega) \times H^1(\Omega) \times H^1_{0,\sigma}(\Omega;\mathbb{R}^N)$ is Lipschitz continuous.*

Proof. For $i = 1, 2$ let $(\varphi_i, \mu_i, v_i) \in \tilde{S}_{\overline{\Psi}}(u_i)$ and $a_i \in \partial\overline{\Psi}_0(\varphi_i)$ be the associated slack variable. Then it holds that

$$\left\langle \frac{\varphi_1 - \varphi_2}{\tau}, \phi \right\rangle + \langle (v_1 - v_2)\nabla\varphi_{-1}, \phi\rangle + (m(\varphi_{-1})\nabla(\mu_1 - \mu_2), \nabla\phi) = 0, \tag{5.35a}$$

$$(\nabla(\varphi_1 - \varphi_2), \nabla\phi) + \langle a_1 - a_2, \phi\rangle - \langle \mu_1 - \mu_2, \phi\rangle = 0, \tag{5.35b}$$

$$\begin{aligned} \left\langle \frac{\rho(\varphi_{-1})(v_1 - v_2)}{\tau}, \psi \right\rangle_{H^{-1}_{0,\sigma}, H^1_{0,\sigma}} &- ((v_1 - v_2) \otimes \rho(\varphi_{-2})v_{-1}, \nabla\psi) \\ + \left((v_1 - v_2) \otimes \frac{\rho_2 - \rho_1}{2} m(\varphi_{-2})\nabla\mu_{-1}, \nabla\psi \right) &+ (2\eta(\varphi_{-1})\varepsilon(v_1 - v_2), \varepsilon(\psi)) \\ - \langle (\mu_1 - \mu_2)\nabla\varphi_{-1}, \psi\rangle_{H^{-1}_{0,\sigma}, H^1_{0,\sigma}} &- \langle u_1 - u_2, \psi\rangle_{H^{-1}_{0,\sigma}, H^1_{0,\sigma}} = 0. \end{aligned} \tag{5.35c}$$

Testing these equations with $\tau(\mu_1 - \mu_2)$, $(\varphi_1 - \varphi_2)$ and $\tau(v_1 - v_2)$, respectively, and summing up, we obtain

$$\begin{aligned} &\int_\Omega \rho(\varphi_{-1})|v_1 - v_2|^2 dx + \tau \int_\Omega \operatorname{div} v \frac{|v_1 - v_2|^2}{2} dx \\ &+ 2\tau \int_\Omega \eta(\varphi_{-1})|\varepsilon(v_1 - v_2)|^2 dx + \tau \int_\Omega m(\varphi_{-1})|\nabla(\mu_1 - \mu_2)|^2 dx \\ &+ \int_\Omega |\nabla(\varphi_1 - \varphi_2)|^2 dx + \langle a_1 - a_2, \varphi_1 - \varphi_2\rangle \\ &= \tau \langle u_1 - u_2, v_1 - v_2\rangle_{H^{-1}_{0,\sigma}, H^1_{0,\sigma}}, \end{aligned}$$

where we additionally employed the relations (2.53) and (5.14). With the help of equation (5.2) this leads to

$$\begin{aligned} &\int_\Omega \frac{\rho(\varphi_{-1}) + \rho(\varphi_{-2})}{2} |v_1 - v_2|^2 dx + 2\tau \int_\Omega \eta(\varphi_{-1})|\varepsilon(v_1 - v_2)|^2 dx \\ &+ \tau \int_\Omega m(\varphi_{-1})|\nabla(\mu_1 - \mu_2)|^2 dx + \int_\Omega |\nabla(\varphi_1 - \varphi_2)|^2 dx + \langle a_1 - a_2, \varphi_1 - \varphi_2\rangle \\ &= \tau \langle u_1 - u_2, v_1 - v_2\rangle_{H^{-1}_{0,\sigma}, H^1_{0,\sigma}}. \end{aligned}$$

Due to the monotonicity of $\partial\overline{\Psi}$, the non-negativity of ρ, and the boundedness of m and η, this yields

$$\begin{aligned} C_1\|\nabla(v_1 - v_2)\|^2 + C_2\|\nabla(\mu_1 - \mu_2)\|^2 + \|\nabla(\varphi_1 - \varphi_2)\|^2 \\ \leq \tau\|u_1 - u_2\|_{H^{-1}_{0,\sigma}}\|v_1 - v_2\|_{H^1}, \end{aligned} \tag{5.36}$$

where $C_1, C_2 > 0$ are positive constants depending on τ, η, and m.

By testing (5.35a) with $\phi \equiv 1$, we further derive

$$0 = \frac{1}{\tau}\int_\Omega \varphi_1(x) - \varphi_2(x)dx + \int_\Omega (v_1(x) - v_2(x))\nabla\varphi_{-1}(x)dx \tag{5.37}$$

$$= \frac{1}{\tau}\left(\int_\Omega \varphi_1(x) - \varphi_2(x)dx\right), \tag{5.38}$$

where we took advantage of the fact that $v_1 - v_2$ is an element of $H^1_{0,\sigma}(\Omega;\mathbb{R}^N)$. In combination with Poincaré's inequality, Korn's inequality and (5.36) this verifies the existence of a constant C such that

$$\|v_1 - v_2\|^2_{H^1} + \|\nabla(\mu_1 - \mu_2)\|^2 + \|\varphi_1 - \varphi_2\|^2_{H^1} \leq C\|u_1 - u_2\|_{H^{-1}_{0,\sigma}}\|v_1 - v_2\|_{H^1}. \tag{5.39}$$

Hence

$$\|\varphi_1 - \varphi_2\|_{H^1} \leq C\|u_1 - u_2\|_{H^{-1}}. \tag{5.40}$$

By Sobolev's Embedding Theorem 1.2.1 $\varphi_1, \varphi_2 \in H^2(\Omega)$ are contained in the Hölder space $C^\alpha(\overline{\Omega})$ for some $\alpha > 0$. This implies the existence of a constant C_1 such that

$$\|\varphi_1 - \varphi_2\|_C = \max_{x\in\overline{\Omega}}\{|\varphi_1(x) - \varphi_2(x)|\} \leq C_1\|u_1 - u_2\|_{H^{-1}}. \tag{5.41}$$

To see this we define $x_{max} \in \overline{\Omega}$ and $\delta_{max} > 0$ such that

$$\delta_{max} := \|\varphi_1 - \varphi_2\|_C = \varphi_1(x_{max}) - \varphi_2(x_{max}). \tag{5.42}$$

Due to the Hölder continuity of $\varphi_1 - \varphi_2$, there exists a neighborhood $x_{max} \in \Omega_{x_{max}} \subset \overline{\Omega}$ with positive measure such that $\varphi_1(x) - \varphi_2(x) > \frac{\delta_{max}}{2}$ for all $x \in \Omega_{x_{max}}$. Consequently, inequality (5.41) holds true, since

$$\|\varphi_1 - \varphi_2\|_C \frac{|\Omega_{x_{max}}|}{2} = \frac{\delta_{max}}{2}|\Omega_{x_{max}}| \leq \|\varphi_1 - \varphi_2\|_{H^1}. \tag{5.43}$$

Next, we observe that there exists a $\delta > 0$ and a subset $\Omega_\delta \subset \Omega$ with positive measure such that $-1 + \delta < \varphi_1(x) < 1 - \delta$ a.e. on Ω_δ. The estimate (5.41) ensures that $\|\varphi_1 - \varphi_2\|_C \leq \delta$, if $\|u_1 - u_2\|_{H^{-1}}$ is sufficiently small. As a consequence, it holds that $-1 < \varphi_2(x) < 1$ a.e. on Ω_δ.

Due to the characterization of the subdifferential of the double-obstacle potential, this implies

$$a_1 = a_2 = 0 \text{ a.e. on } \Omega_\delta. \tag{5.44}$$

Employing equation (5.35b), we infer

$$\mu_1 - \mu_2 = -\Delta(\varphi_1 - \varphi_2) + a_1 - a_2 = -\Delta(\varphi_1 - \varphi_2), \text{ a.e. on } \Omega_\delta. \tag{5.45}$$

Let us define the mean value of $\mu_1 - \mu_2$ by $\tilde{c}_\mu := \frac{1}{|\Omega|}\int_\Omega \mu_1 - \mu_2 dx$ and $\tilde{w}_\mu := \mu_1 - \mu_2 - \tilde{c}_\mu$. Clearly, the mean value of $\tilde{w}_\mu$ is equal to zero and Poincaré's inequality yields

$$\int_{\Omega_\delta} \tilde{w}_\mu dx \leq \int_{\Omega_\delta} |\tilde{w}_\mu| dx \leq \|\tilde{w}_\mu\|_{L^1} \leq C\|\nabla \tilde{w}_\mu\| = C\|\nabla(\mu_1 - \mu_2)\|. \tag{5.46}$$

With the help of the divergence theorem we derive

$$|\tilde{c}_\mu||\Omega_\delta| = \left|\int_{\Omega_\delta} \tilde{c}_\mu dx\right| = \left|\int_{\Omega_\delta} -\Delta(\varphi_1 - \varphi_2) dx - \int_{\Omega_\delta} \tilde{w}_\mu dx\right| \tag{5.47}$$

$$= \left|\int_{\partial\Omega_\delta} \nabla(\varphi_1 - \varphi_2)\vec{n} dx - \int_{\Omega_\delta} \tilde{w}_\mu dx\right| \tag{5.48}$$

$$\leq C(\|\varphi_1 - \varphi_2\|_{H^1} + \|\nabla(\mu_1 - \mu_2)\|). \tag{5.49}$$

In combination with (5.39) and Poincaré's inequality with respect to $\mu_1 - \mu_2$, this yields the assertion. $\square$

Note that Theorem 5.1.1 and (5.34b) imply that the difference of the slack variables a_1, a_2 from the above proof is bounded in $H^1(\Omega)^*$, i.e.

$$\|a_1 - a_2\|^2_{H^{-1}} \leq C\|u_1 - u_2\|^2_{H^{-1}_{0,\sigma}}. \tag{5.50}$$

Another immediate consequence of Theorem 5.1.1 is that the solutions to the discretized Cahn-Hilliard-Navier-Stokes system (5.3) are uniquely determined by the control u.

5.1.2 Directional differentiability

In this section we derive a characterization of the directional derivative of the constraint mapping $\tilde{S}_{\overline{\Psi}}$. The proof utilizes some of the variational concepts introduced in Section 1.3.

Employing the notation from Definition 3.3.1, we rewrite the variational inequality (5.34b) as a complementarity problem

$$\left\langle a^+ + a^-, \phi \right\rangle = \langle \nabla\varphi, \nabla\phi \rangle - \langle \mu, \phi \rangle, \ \forall \phi \in H^1(\Omega), \tag{5.51}$$

$$\left\langle a^-, \varphi - \psi_2 \right\rangle = 0, \ \left\langle a^+, \varphi - \psi_1 \right\rangle = 0, \tag{5.52}$$

$$\left\langle a^+, \phi_2 \right\rangle \geq 0, \ \left\langle a^-, \phi_2 \right\rangle \leq 0, \ \forall \phi_2 \in H^1(\Omega) : \phi_2 \geq 0 \text{ a.e. on } \Omega. \tag{5.53}$$

Then the directional derivative of $\tilde{S}_{\overline{\Psi}}$ is given by the subsequent theorem.

Theorem 5.1.2. *The directional derivative of the control-to-state operator $\tilde{S}_{\overline{\Psi}}$ at $u_0 \in H^1_{0,\sigma}(\Omega;\mathbb{R}^N)^*$, with $\tilde{S}_{\overline{\Psi}}(u_0) = (\varphi_0, \mu_0, v_0)$ and the associated slack variable $a_0 \in \partial\overline{\Psi}_0(\varphi_0)$, in the direction $h \in H^1_{0,\sigma}(\Omega;\mathbb{R}^N)^*$ is given by $D\tilde{S}_{\overline{\Psi}}[u_0](h) = (q, w, \zeta)$, where $(q, w, \zeta) \in H^1(\Omega) \times H^1(\Omega) \times H^1_{0,\sigma}(\Omega;\mathbb{R}^N)$ is the unique solution to the system*

$$q \in T_{\mathbb{K}}(\varphi_0) \cap \{a_0^+\}^\perp \cap \{a_0^-\}^\perp, \tag{5.54a}$$
$$\left\langle -\Delta q - w, \tilde{\phi} - q \right\rangle \geq 0,\ \forall \tilde{\phi} \in T_{\mathbb{K}}(\varphi_0) \cap \{a_0^+\}^\perp \cap \{a_0^-\}^\perp, \tag{5.54b}$$
$$\left\langle \frac{q}{\tau}, \phi \right\rangle + \langle \zeta \nabla \varphi_{-1}, \phi \rangle + (m(\varphi_{-1}) \nabla w, \nabla \phi) = 0, \tag{5.54c}$$
$$\begin{aligned}\left\langle \frac{\rho(\varphi_{-1})\zeta}{\tau}, \psi \right\rangle_{H^{-1}_{0,\sigma}, H^1_{0,\sigma}} &- (\zeta \otimes \rho(\varphi_{-2}) v_{-1}, \nabla \psi) \\ + \left(\zeta \otimes \frac{\rho_2 - \rho_1}{2} m(\varphi_{-2}) \nabla \mu_{-1}, \nabla \psi \right) &+ (2\eta(\varphi_{-1}) \varepsilon(\zeta), \varepsilon(\psi)) \\ - \langle w \nabla \varphi_{-1}, \psi \rangle_{H^{-1}_{0,\sigma}, H^1_{0,\sigma}} &= \langle h, \psi \rangle_{H^{-1}_{0,\sigma}, H^1_{0,\sigma}}.\end{aligned} \tag{5.54d}$$

Proof. For $\theta > 0$ we consider $u_\theta := u_0 + \theta h \in H^1_{0,\sigma}(\Omega;\mathbb{R}^N)^*$, $(\varphi_\theta, \mu_\theta, v_\theta) := \tilde{S}_{\overline{\Psi}}(u_\theta)$, and the associated slack variables $a_\theta := a_\theta^+ + a_\theta^-$.

Due to the Lipschitz continuity of $\tilde{S}_{\overline{\Psi}}$ and (5.50), the sets

$$\{\frac{\varphi_\theta - \varphi_0}{\theta} : 0 < \theta \leq 1\}, \{\frac{\mu_\theta - \mu_0}{\theta} : 0 < \theta \leq 1\} \in H^1(\Omega), \tag{5.55}$$
$$\{\frac{v_\theta - v_0}{\theta} : 0 < \theta \leq 1\} \in H^1_{0,\sigma}(\Omega;\mathbb{R}^N), \tag{5.56}$$
$$\{\frac{a_\theta^+ - a_0^+}{\theta} : 0 < \theta \leq 1\}, \{\frac{a_\theta^- - a_0^-}{\theta} : 0 < \theta \leq 1\} \in H^1(\Omega)^*, \tag{5.57}$$

are bounded in the respective spaces. Consequently, there exists a sequence $\theta_k \to 0$ such that the associated subsequences converge weakly towards weak limit points denoted by q, w, ζ, Ξ^+, Ξ^-, i.e.

$$\frac{\varphi_{\theta_k} - \varphi_0}{\theta_k} \rightharpoonup q, \quad \frac{\mu_{\theta_k} - \mu_0}{\theta_k} \rightharpoonup w, \quad \frac{v_{\theta_k} - v_0}{\theta_k} \rightharpoonup \zeta,$$
$$\frac{a_{\theta_k}^+ - a_0^+}{\theta_k} \rightharpoonup \Xi^+, \quad \frac{a_{\theta_k}^- - a_0^-}{\theta_k} \rightharpoonup \Xi^-,$$

for $k \to \infty$.

Next, we consider the system (5.35) for $u_1 := u_{\theta_k}$ and $u_2 := u_0$. We multiply the system by $\frac{1}{\theta_k}$ and pass to the limit for $k \to \infty$. In this process we utilize the convergence and embedding arguments from the proof of Theorem 3.2.1 to obtain

$$\langle \nabla q, \nabla \phi \rangle - \langle w, \phi \rangle - \langle \Xi, \phi \rangle = 0 \tag{5.58a}$$

$$\left\langle \frac{q}{\tau}, \phi \right\rangle + \langle \zeta \nabla \varphi_{-1}, \phi \rangle + (m(\varphi_{-1}) \nabla w, \nabla \phi) = 0, \tag{5.58b}$$

$$\begin{aligned} \left\langle \frac{\rho(\varphi_{-1})\zeta}{\tau}, \psi \right\rangle_{H^{-1}_{0,\sigma}, H^1_{0,\sigma}} &- (\zeta \otimes \rho(\varphi_{-2}) v_{-1}, \nabla \psi) \\ + \left(\zeta \otimes \frac{\rho_2 - \rho_1}{2} m(\varphi_{-2}) \nabla \mu_{-1}, \nabla \psi \right) &+ (2\eta(\varphi_{-1}) \varepsilon(\zeta), \varepsilon(\psi)) \\ - \langle w \nabla \varphi_{-1}, \psi \rangle_{H^{-1}_{0,\sigma}, H^1_{0,\sigma}} &- \langle h, \psi \rangle_{H^{-1}_{0,\sigma}, H^1_{0,\sigma}} = 0, \end{aligned} \tag{5.58c}$$

where $\Xi := \Xi^+ + \Xi^-$. Let us exemplary show the convergence of the term $\left(\frac{v_{\theta_k} - v_0}{\theta_k} \otimes \frac{\rho_2 - \rho_1}{2} m(\varphi_{-2}) \nabla \mu_{-1}, \nabla \psi \right)$. By Hölder's inequality it holds that

$$\| m(\varphi_{-2}) \nabla \mu_{-1} \cdot \nabla \psi \|_{L^{4/3}} \leq \| m(\varphi_{-2}) \|_{L^\infty} \| \nabla \mu_{-1} \|_{L^4} \| \nabla \psi \|_{L^2}. \tag{5.59}$$

Employing Sobolev's Embedding Theorem 1.2.1 and the weak continuity of the embedding operator, it can be verified that $\frac{v_{\theta_k} - v_0}{\theta_k}$ converges weakly to ζ in $L^4(\Omega)$. In summary, this leads to

$$\begin{aligned} &\lim_{k \to \infty} \left\langle \frac{v_{\theta_k} - v_0}{\theta_k} \otimes \frac{\rho_2 - \rho_1}{2} m(\varphi_{-2}) \nabla \mu_{-1}, \nabla \psi \right\rangle \\ &\qquad = \left\langle \zeta \otimes \frac{\rho_2 - \rho_1}{2} m(\varphi_{-2}) \nabla \mu_{-1}, \nabla \psi \right\rangle. \end{aligned} \tag{5.60}$$

The convergence of the remaining terms in the system (5.58) is shown analogously. Note that this already ensures that the equations (5.54c) and (5.54d) are satisfied.

The rest of the proof is split into three separate lemmata which further characterize the directional derivative associated to the variational inequality (5.34b).

Lemma 5.1.2. *Let Ξ^+ and Ξ^- be weak limit points of $\frac{a^+_{\theta_k} - a^+_0}{\theta_k}$ and $\frac{a^-_{\theta_k} - a^-_0}{\theta_k}$ as defined above. Then it holds for all $\phi \in T_{\mathbb{K}}(\varphi_0) \cap \{a^+_0\}^\perp \cap \{a^-_0\}^\perp$ that*

$$\langle \Xi, \phi \rangle = \langle \Xi^+ + \Xi^-, \phi \rangle \geq 0. \tag{5.61}$$

Proof. By (5.53) it holds for arbitrary $k \in \mathbb{N}$ that

$$\left\langle -a_0^-, (\varphi_{\theta_k} - \psi_2) \right\rangle \leq 0 \quad \wedge \quad \left\langle a_{\theta_k}^-, -(\varphi_0 - \psi_2) \right\rangle \leq 0. \tag{5.62}$$

In combination with (5.52) this leads to

$$\left\langle a_{\theta_k}^- - a_0^-, \varphi_{\theta_k} - \varphi_0 \right\rangle = \left\langle a_{\theta_k}^- - a_0^-, (\varphi_{\theta_k} - \psi_2) - (\varphi_0 - \psi_2) \right\rangle \tag{5.63}$$

$$= \left\langle a_{\theta_k}^-, -(\varphi_0 - \psi_2) \right\rangle + \left\langle -a_0^-, (\varphi_{\theta_k} - \psi_2) \right\rangle \leq 0. \tag{5.64}$$

Using the Lipschitz continuity of $\tilde{S}_{\overline{\Psi}}$ and (5.50), we infer

$$\left| \left\langle a_{\theta_k}^-, -(\varphi_0 - \psi_2) \right\rangle \right| \leq \left| \left\langle a_{\theta_k}^- - a_0^-, \varphi_{\theta_k} - \varphi_0 \right\rangle \right| \tag{5.65}$$

$$\leq \left| \left\langle a_{\theta_k} - a_0, \varphi_{\theta_k} - \varphi_0 \right\rangle \right| \tag{5.66}$$

$$\leq C \left\| u_1 - u_2 \right\|_{H_{0,\sigma}^{-1}}^2 \tag{5.67}$$

$$\leq C \theta_k^2 \left\| h \right\|_{H_{0,\sigma}^{-1}}^2. \tag{5.68}$$

Hence

$$\left\langle \Xi^-, \varphi_0 - \psi_2 \right\rangle = \lim_{k\to\infty} \left\langle \frac{a_{\theta_k}^- - a_0^-}{\theta_k}, \varphi_0 - \psi_2 \right\rangle = \lim_{k\to\infty} \left\langle \frac{a_{\theta_k}^-}{\theta_k}, \varphi_0 - \psi_2 \right\rangle = 0. \tag{5.69}$$

Analogously, it is shown that

$$\left\langle \Xi^+, \varphi_0 - \psi_1 \right\rangle = 0. \tag{5.70}$$

Since $\mathbb{K}$ is convex and polyhedric, cf. [148], it holds that

$$T_{\mathbb{K}}(\varphi_0) \cap \{a_0^+\}^\perp \cap \{a_0^-\}^\perp = \overline{R_{\mathbb{K}}(\varphi_0) \cap \{a_0^+\}^\perp \cap \{a_0^-\}^\perp}, \tag{5.71}$$

see Definition 1.3.3. We therefore consider an arbitrary $\phi \in R_{\mathbb{K}}(\varphi_0) \cap \{a_0^-\}^\perp \cap \{a_0^+\}^\perp$. By the definition of the radial cone there exists a $\bar{t} > 0$ such that $\varphi_0 + \bar{t}\phi \in \mathbb{K}$, which implies that

$$\varphi_0 + \bar{t}\phi - \psi_2 \leq 0 \text{ a.e. on } \Omega. \tag{5.72}$$

Due to (5.52), $\varphi_0 + \bar{t}\phi - \psi_2$ is contained in $\{a_0^-\}^\perp$ and it holds that

$$\left\langle \Xi^-, \varphi_0 + \bar{t}\phi - \psi_2 \right\rangle = \lim_{k\to\infty} \left\langle \frac{a_{\theta_k}^- - a_0^-}{\theta_k}, \varphi_0 + \bar{t}\phi - \psi_2 \right\rangle \tag{5.73}$$

$$= \lim_{k\to\infty} \left\langle \frac{a_{\theta_k}^-}{\theta_k}, \varphi_0 + \bar{t}\phi - \psi_2 \right\rangle \tag{5.74}$$

With the help of (5.53) and (5.72) we infer

$$\left\langle \Xi^-, \varphi_0 + \bar{t}\phi - \psi_2 \right\rangle = \lim_{k\to\infty} \left\langle \frac{a^-_{\theta_k}}{\theta_k}, \varphi_0 + \bar{t}\phi - \psi_2 \right\rangle \geq 0.$$

In combination with (5.69) this yields

$$\left\langle \Xi^-, \phi \right\rangle \geq 0. \tag{5.75}$$

Analogously, it is verified that $\langle \Xi^+, \phi \rangle \geq 0$, which leads to

$$\langle \Xi, \phi \rangle = \left\langle \Xi^+ + \Xi^-, \phi \right\rangle \geq 0, \tag{5.76}$$

Since $R_{\mathbb{K}}(\varphi_0) \cap \{a_0^-\}^\perp \cap \{a_0^+\}^\perp$ is a dense subset of $T_{\mathbb{K}}(\varphi_0) \cap \{a_0^+\}^\perp \cap \{a_0^-\}^\perp$, this proves the assertion. □

Lemma 5.1.3. *Let q be a weak limit of $\frac{\varphi_{\theta_k} - \varphi_0}{\theta_k}$ as defined above. Then q is an element of the critical cone, i.e.*

$$q \in T_{\mathbb{K}}(\varphi_0) \cap \{a_0^+\}^\perp \cap \{a_0^-\}^\perp. \tag{5.77}$$

Proof. By the definition of the tangent cone, q is contained in $T_{\mathbb{K}}(\varphi_0)$. It remains to be shown that q is orthogonal to a_0^+ and a_0^-. Due to (5.52), it holds that

$$\left\langle a_0^-, q \right\rangle = \lim_{k\to\infty} \left\langle a_0^-, \frac{\varphi_{\theta_k} - \varphi_0}{\theta_k} \right\rangle = \lim_{k\to\infty} \left\langle a_0^-, \frac{\varphi_{\theta_k} - \psi_2}{\theta_k} \right\rangle \geq 0. \tag{5.78}$$

Further note that

$$\lim_{k\to\infty} \left\langle a_0^- - a^-_{\theta_k}, \frac{\varphi_{\theta_k} - \varphi_0}{\theta_k} \right\rangle = 0. \tag{5.79}$$

Consequently,

$$\begin{aligned}
\left\langle a_0^-, q \right\rangle &= \lim_{k\to\infty} \left\langle a_0^-, \frac{\varphi_{\theta_k} - \varphi_0}{\theta_k} \right\rangle && (5.80)\\
&= \lim_{k\to\infty} \left(\left\langle a^-_{\theta_k}, \frac{\varphi_{\theta_k} - \varphi_0}{\theta_k} \right\rangle + \left\langle a_0^- - a^-_{\theta_k}, \frac{\varphi_{\theta_k} - \varphi_0}{\theta_k} \right\rangle \right) && (5.81)\\
&= \lim_{k\to\infty} \left\langle a^-_{\theta_k}, \frac{\varphi_{\theta_k} - \varphi_0}{\theta_k} \right\rangle = \lim_{k\to\infty} \left\langle a^-_{\theta_k}, \frac{-(\varphi_0 - \psi_2)}{\theta_k} \right\rangle \leq 0. && (5.82)
\end{aligned}$$

In combination with (5.78), this leads to

$$\left\langle a_0^-, q \right\rangle = 0. \tag{5.83}$$

Analogously, we derive $\left\langle a_0^+, q \right\rangle = 0$. □

Lemma 5.1.4. *Let q and Ξ be weak limit points of $\frac{\varphi_{\theta_k}-\varphi_0}{\theta_k}$ and $\frac{a_{\theta_k}-a_0}{\theta_k}$ as defined above. Then it holds that*

$$\langle \Xi, q\rangle = 0. \tag{5.84}$$

Proof. Let us define the linear operator $D : H^1(\Omega)\times H^1_{0,\sigma}(\Omega;\mathbb{R}^N) \to H^1(\Omega)^* \times H^1_{0,\sigma}(\Omega;\mathbb{R}^N)^*$ by

$$D(\mu,v) := \begin{pmatrix} v\nabla\varphi_{-1} - \operatorname{div}(m(\varphi_{-1})\nabla\mu) \\ \frac{\rho(\varphi_{-1})v}{\tau} + \operatorname{div}(v\otimes v) - \operatorname{div}(2\eta(\varphi_{-1})\varepsilon(v)) - \mu\nabla\varphi_{-1} \end{pmatrix}. \tag{5.85}$$

First, we show that D is invertible, i.e. for every pair $(\Theta_\mu,\Theta_v) \in H^1(\Omega)^* \times H^1_{0,\sigma}(\Omega;\mathbb{R}^N)^*$ there exists a pair $(\mu,v)\in H^1(\Omega)\times H^1_{0,\sigma}(\Omega;\mathbb{R}^N)$ such that for every $\phi\in H^1(\Omega)$ and $\psi \in H^1_{0,\sigma}(\Omega;\mathbb{R}^N)$ it holds that

$$\langle v\nabla\varphi_{-1},\phi\rangle + (m(\varphi_{-1})\nabla\mu,\nabla\phi) = \langle \Theta_\mu,\phi\rangle, \tag{5.86a}$$

$$\begin{aligned} &\left\langle \frac{\rho(\varphi_{-1})v}{\tau},\psi\right\rangle_{H^{-1}_{0,\sigma},H^1_{0,\sigma}} - (v\otimes v,\nabla\psi) \\ &+ (2\eta(\varphi_{-1})\varepsilon(v),\varepsilon(\psi)) - \langle \mu\nabla\varphi_{-1},\psi\rangle_{H^{-1}_{0,\sigma},H^1_{0,\sigma}} = \langle\Theta_v,\psi\rangle_{H^{-1}_{0,\sigma},H^1_{0,\sigma}}. \end{aligned} \tag{5.86b}$$

This is proven by following the same argumentation as in Theorem 5.1.1 (and Theorem 2.2.1). More precisely, the operators $\mathscr{G},\mathscr{F} : H^1(\Omega)\times H^1_{0,\sigma}(\Omega;\mathbb{R}^N) \to H^1(\Omega)^*\times H^1_{0,\sigma}(\Omega;\mathbb{R}^N)^*$ are defined via

$$\begin{aligned} \langle \mathscr{G}_1(\mu),\phi\rangle &:= (m(\varphi_{-1})\nabla\mu,\nabla\phi) + \langle\mu,\phi\rangle - \langle\Theta_\mu,\phi\rangle, \\ \langle \mathscr{G}_2(v),\psi\rangle_{H^{-1}_{0,\sigma},H^1_{0,\sigma}} &:= (2\eta(\varphi_{-1})\varepsilon(v),\varepsilon(\psi)) - \langle\Theta_v,\psi\rangle_{H^{-1}_{0,\sigma},H^1_{0,\sigma}}, \\ \mathscr{F}_1(\mu,v) &:= -v\nabla\varphi_{-1} + \mu, \\ \langle\mathscr{F}_2(\mu,v),\psi\rangle_{H^{-1}_{0,\sigma},H^1_{0,\sigma}} &:= \left\langle -\frac{\rho(\varphi_{-1})v}{\tau} + \mu\nabla\varphi_{-1},\psi\right\rangle_{H^{-1}_{0,\sigma},H^1_{0,\sigma}} + (v\otimes v,\nabla\psi), \end{aligned}$$

and it is verified (by Schaefer's theorem) that the fixed point equation

$$\delta^* - \mathscr{F}\circ\mathscr{G}^{-1}(\delta^*) = 0 \tag{5.87}$$

has a solution $\delta^*\in L^{\frac{3}{2}}(\Omega)\times L^{\frac{3}{2}}(\Omega;\mathbb{R}^N)$. In the process, the boundedness of the solutions $(\mu,v)\in H^1(\Omega)\times H^1_{0,\sigma}(\Omega;\mathbb{R}^N)$ of

$$\mathscr{G}(\mu,v) - \lambda\mathscr{F}(\mu,v) = 0 \tag{5.88}$$

for arbitrary $\lambda \in [0,1]$ is verified by taking advantage of the fact that any solution of (5.88) satisfies the following estimate

$$\begin{aligned}
&\langle \Theta_\mu, \mu\rangle + \langle \Theta_v, v\rangle_{H^{-1}_{0,\sigma},H^1_{0,\sigma}} \\
&= (1-\lambda)\int_\Omega |\mu|^2\,dx + \lambda\int_\Omega \frac{\rho(\varphi_{-1})\,|v|^2}{\tau}dx + \lambda\int_\Omega \frac{\operatorname{div} v\,|v|^2}{2}dx \\
&\quad + \int_\Omega 2\eta(\varphi_{-1})\,|\varepsilon(v)|^2\,dx + \int_\Omega m(\varphi_{-1})\,|\nabla\mu|^2\,dx \\
&\geq (1-\lambda)\int_\Omega |\mu|^2\,dx + \int_\Omega 2\eta(\varphi_{-1})\,|\varepsilon(v)|^2\,dx + \int_\Omega m(\varphi_{-1})\,|\nabla\mu|^2\,dx,
\end{aligned} \tag{5.89}$$

where we used (2.53) and (5.22). Then the invertibility of D follows analogously to the proof of Theorem 5.1.1.

For an arbitrarily chosen $\hat{\varphi} \in H^1(\Omega)$ we define

$$\hat{\mu} := \left[D^{-1}(-\frac{\hat{\varphi}}{\tau},0)\right]_1, \quad \hat{v} := \left[D^{-1}(-\frac{\hat{\varphi}}{\tau},0)\right]_2, \tag{5.90}$$

where $\left[D^{-1}(x)\right]_i$ denotes the i-th component of the linear operator D^{-1} at x. Consequently, it holds for all $\phi \in H^1(\Omega)$ and $\psi \in H^1_{0,\sigma}(\Omega;\mathbb{R}^N)$ that

$$\langle \hat{v}\nabla\varphi_{-1}, \phi\rangle + \langle m(\varphi_{-1})\nabla\hat{\mu}, \nabla\phi\rangle - \left\langle -\frac{\hat{\varphi}}{\tau}, \phi\right\rangle = 0, \tag{5.91a}$$

$$\begin{aligned}
\left\langle \frac{\rho(\varphi_{-1})\hat{v}}{\tau}, \psi\right\rangle_{H^{-1}_{0,\sigma},H^1_{0,\sigma}} &- \langle (\hat{v}\otimes v), \nabla\psi\rangle + (2\eta(\varphi_{-1})\varepsilon(\hat{v}), \varepsilon(\psi)) \\
&- \langle \hat{\mu}\nabla\varphi_{-1}, \psi\rangle_{H^{-1}_{0,\sigma},H^1_{0,\sigma}} = 0.
\end{aligned} \tag{5.91b}$$

By testing (5.91a) and (5.91b) with $\tau\hat{\mu}$ and $\tau\hat{v}$, respectively, and summing up, we obtain

$$\begin{aligned}
0 &\leq \int_\Omega \frac{\rho(\varphi_{-1}) + \rho(\varphi_{-2})}{2}|\hat{v}|^2 dx + 2\tau\int_\Omega \eta(\varphi_{-1})|\varepsilon(\hat{v})|^2 dx \\
&\quad + \tau\int_\Omega m(\varphi_{-1})|\nabla(\hat{\mu})|^2 dx \\
&= -\langle \hat{\mu}, \hat{\varphi}\rangle,
\end{aligned} \tag{5.92}$$

where we additionally used the condition (5.2) once again. Hence

$$\left\langle \left[D^{-1}(-\frac{\hat{\varphi}}{\tau},0)\right]_1, \hat{\varphi}\right\rangle \leq 0. \tag{5.93}$$

As a consequence, the linear operator $\mathscr{B} : H^1(\Omega) \to H^1(\Omega)^*$ defined by

$$\mathscr{B}(\hat{\varphi}) := -\Delta\hat{\varphi} - \left[D^{-1}(-\frac{\hat{\varphi}}{\tau}, 0) \right]_1 , \tag{5.94}$$

is coercive in the sense that

$$\langle \mathscr{B}(\hat{\varphi}), \hat{\varphi} \rangle = \|\nabla\hat{\varphi}\|_{L^2}^2 - \left\langle \left[D^{-1}(-\frac{\hat{\varphi}}{\tau}, 0) \right]_1 , \hat{\varphi} \right\rangle \geq \|\nabla\hat{\varphi}\|_{L^2}^2 \geq 0. \tag{5.95}$$

Moreover, for every $\theta > 0$, it holds that

$$\mathscr{B}(\varphi_\theta) = -\Delta\varphi_\theta - \left[D^{-1}(-\frac{\varphi_\theta}{\tau}, 0) \right]_1 = a_\theta + \mu_\theta - \left[D^{-1}(-\frac{\varphi_\theta}{\tau}, 0) \right]_1 , \tag{5.96}$$

due to equation (5.34b). Employing the equations (5.34a) and (5.34c) we infer

$$D(\mu_\theta, v_\theta) = \begin{pmatrix} -\frac{\varphi_\theta - \varphi_{-1}}{\tau} - \kappa \mathrm{div}(m(\varphi_{-1})\nabla\varphi_{-1}) \\ \frac{\rho(\varphi_{-2})v_{-1}}{\tau} + u_\theta - \kappa\varphi_{-1}\nabla\varphi_{-1} \end{pmatrix}, \tag{5.97}$$

which leads to

$$(\mu_\theta, v_\theta) - D^{-1}(-\frac{\varphi_\theta}{\tau}, 0) = D^{-1} \begin{pmatrix} \frac{\varphi_{-1}}{\tau} - \kappa \mathrm{div}(m(\varphi_{-1})\nabla\varphi_{-1}) \\ \frac{\rho(\varphi_{-2})v_{-1}}{\tau} + u_\theta - \kappa\varphi_{-1}\nabla\varphi_{-1} \end{pmatrix}. \tag{5.98}$$

Hence

$$\mathscr{B}(\varphi_\theta) = a_\theta + \mu_\theta - \left[D^{-1}(-\frac{\varphi_\theta}{\tau}, 0) \right]_1 \tag{5.99}$$

$$= a_\theta + \left[D^{-1} \begin{pmatrix} \frac{\varphi_{-1}}{\tau} - \kappa \mathrm{div}(m(\varphi_{-1})\nabla\varphi_{-1}) \\ \frac{\rho(\varphi_{-2})v_{-1}}{\tau} + u_\theta - \kappa\varphi_{-1}\nabla\varphi_{-1} \end{pmatrix} \right]_1 . \tag{5.100}$$

Due to the linearity of $\mathscr{B}$ and D^{-1}, this yields (for $\theta > 0$)

$$\mathscr{B}(\frac{\varphi_\theta - \varphi_0}{\theta}) = \frac{1}{\theta} \left(a_\theta - a_0 + \left[D^{-1} \begin{pmatrix} 0 \\ u_\theta - u_0 \end{pmatrix} \right]_1 \right) \tag{5.101}$$

$$= \frac{a_\theta - a_0}{\theta} + \left[D^{-1} \begin{pmatrix} 0 \\ h \end{pmatrix} \right]_1 . \tag{5.102}$$

In order to simplify the notation we subsequently introduce the linear operator

$$\hat{D}(h) := \left[D^{-1} \begin{pmatrix} 0 \\ h \end{pmatrix} \right]_1 . \tag{5.103}$$

Taking advantage of (5.95), we derive

$$\frac{1}{2}(\langle\mathscr{B}(z),y\rangle+\langle\mathscr{B}(y),z\rangle)\leq\langle\mathscr{B}(z),z\rangle^{\frac{1}{2}}\langle\mathscr{B}(y),y\rangle^{\frac{1}{2}},\ \forall y,z\in H^1(\Omega). \quad (5.104)$$

For arbitrary $\theta_1,\theta_2>0$ we set $z:=\frac{\varphi_{\theta_1}-\varphi_0}{\theta_1}$ and $y:=\frac{\varphi_{\theta_2}-\varphi_0}{\theta_2}$ and employ equation (5.102) to conclude that

$$\begin{aligned}&\frac{1}{2}\left(\left\langle\frac{a_{\theta_1}-a_0}{\theta_1}+\hat{D}(h),\frac{\varphi_{\theta_2}-\varphi_0}{\theta_2}\right\rangle+\left\langle\frac{a_{\theta_2}-a_0}{\theta_2}+\hat{D}(h),\frac{\varphi_{\theta_1}-\varphi_0}{\theta_1}\right\rangle\right)\\&\quad\leq\left\langle\frac{a_{\theta_1}-a_0}{\theta_1}+\hat{D}(h),\frac{\varphi_{\theta_1}-\varphi_0}{\theta_1}\right\rangle^{\frac{1}{2}}\left\langle\frac{a_{\theta_2}-a_0}{\theta_2}+\hat{D}(h),\frac{\varphi_{\theta_2}-\varphi_0}{\theta_2}\right\rangle^{\frac{1}{2}}.\end{aligned}$$

Due to the monotonicity of $\partial\overline{\Psi}_0$, this yields

$$\begin{aligned}&\frac{1}{2}\left(\left\langle\frac{a_{\theta_1}-a_0}{\theta_1}+\hat{D}(h),\frac{\varphi_{\theta_2}-\varphi_0}{\theta_2}\right\rangle+\left\langle\frac{a_{\theta_2}-a_0}{\theta_2}+\hat{D}(h),\frac{\varphi_{\theta_1}-\varphi_0}{\theta_1}\right\rangle\right)\\&\quad\leq\left\langle\hat{D}(h),\frac{\varphi_{\theta_1}-\varphi_0}{\theta_1}\right\rangle^{\frac{1}{2}}\left\langle\hat{D}(h),\frac{\varphi_{\theta_2}-\varphi_0}{\theta_2}\right\rangle^{\frac{1}{2}}. \qquad (5.105)\end{aligned}$$

By setting $\theta_1:=\theta_k$ and passing to the limit for $k\to\infty$, we verify that the following estimate holds for every $\theta_2>0$

$$\begin{aligned}&\frac{1}{2}\left(\left\langle\Xi+\hat{D}(h),\frac{\varphi_{\theta_2}-\varphi_0}{\theta_2}\right\rangle+\left\langle\frac{a_{\theta_2}-a_0}{\theta_2}+\hat{D}(h),q\right\rangle\right)\\&\quad\leq\left\langle\hat{D}(h),q\right\rangle^{\frac{1}{2}}\left\langle\hat{D}(h),\frac{\varphi_{\theta_2}-\varphi_0}{\theta_2}\right\rangle^{\frac{1}{2}}. \qquad (5.106)\end{aligned}$$

Next, we set $\theta_2:=\theta_k$ and pass to the limit for $k\to\infty$ to obtain

$$\frac{1}{2}\left(\left\langle\Xi+\hat{D}(h),\hat{q}\right\rangle+\left\langle\hat{\Xi}+\hat{D}(h),q\right\rangle\right)\leq\left\langle\hat{D}(h),q\right\rangle^{\frac{1}{2}}\left\langle\hat{D}(h),\hat{q}\right\rangle^{\frac{1}{2}}, \qquad (5.107)$$

where q,Ξ and $\hat{q},\hat{\Xi}$ might be different weak limit points. However, employing Lemma 5.1.2 and Lemma 5.1.3, we infer

$$\begin{aligned}\frac{1}{2}(\left\langle\Xi+\hat{D}(h),\hat{q}\right\rangle+\left\langle\hat{\Xi}+\hat{D}(h),q\right\rangle)&\geq\frac{1}{2}(\left\langle\hat{D}(h),\hat{q}\right\rangle+\left\langle\hat{D}(h),q\right\rangle)\\&\geq\left\langle\hat{D}(h),q\right\rangle^{\frac{1}{2}}\left\langle\hat{D}(h),\hat{q}\right\rangle^{\frac{1}{2}}. \qquad (5.108)\end{aligned}$$

In combination with (5.107) this leads to

$$\frac{1}{2}(\left\langle\Xi+\hat{D}(h),\hat{q}\right\rangle+\left\langle\hat{\Xi}+\hat{D}(h),q\right\rangle)=\frac{1}{2}(\left\langle\hat{D}(h),\hat{q}\right\rangle+\left\langle\hat{D}(h),q\right\rangle) \qquad (5.109)$$

Hence, for all weak limit points $\hat{\Xi}$ and q it holds that

$$\left\langle \hat{\Xi}, q \right\rangle = 0 = \left\langle \Xi, \hat{q} \right\rangle, \tag{5.110}$$

which proves the assertion. □

Combining the three lemmata and taking (5.58a) into account, we infer that every weak limit point q of $\left\{ \frac{\varphi_{\theta_k} - \varphi_0}{\theta_k} \right\}_{k \in \mathbb{N}}$ satisfies the variational inequality

$$q \in T_{\mathbb{K}}(\varphi_0) \cap \{a_0^+\}^{\perp} \cap \{a_0^-\}^{\perp}, \tag{5.111a}$$

$$\left\langle -\Delta q - w, \tilde{\phi} - q \right\rangle \geq 0, \ \forall \tilde{\phi} \in T_{\mathbb{K}}(\varphi_0) \cap \{a_0^+\}^{\perp} \cap \{a_0^-\}^{\perp}. \tag{5.111b}$$

Since the variational inequality (5.111) has a unique solution, this concludes the proof of Theorem 5.1.2. □

According to the above theorem, the directional derivative of the solution operator $\tilde{S}_{\overline{\Psi}}$ itself can be determined as the solution of a coupled system of partial differential equations including a variational inequality, where the corresponding constraint set is represented by the critical cone with respect to $\mathbb{K}$.

5.1.3 Strong stationarity conditions

In this subsection, we present the main result of this section. Based on the directional derivative of $\tilde{S}_{\overline{\Psi}}$ a modified stationarity system for the control problem (I_Ψ) is derived, which enhances the system from Corollary 5.1.4 by the conditions (5.112e) and (5.112f) below.

Theorem 5.1.3. *Let $(\varphi_0, \mu_0, v_0, u_0) \in \tilde{\mathscr{X}}$ be a minimizer of (I_Ψ) with the associated slack variable $a_0 \in \partial\overline{\Psi}_0(\varphi_0)$.*

Then there exists an adjoint state $(p, r, s) \in H^1(\Omega) \times H^1(\Omega) \times H^1_{0,\sigma}(\Omega; \mathbb{R}^N)$

and $\lambda \in H^1(\Omega)^*$ such that for all $\phi \in H^1(\Omega)$ and $\psi \in H^1_{0,\sigma}(\Omega;\mathbb{R}^N)$ it holds that

$$\left\langle D_\varphi \mathscr{J}[z_0] + \frac{r}{\tau}, \phi \right\rangle + (\nabla p, \nabla \phi) + \langle \lambda, \phi \rangle = 0, \quad (5.112a)$$

$$(m(\varphi_{-1})\nabla r, \nabla \phi) - \langle p, \phi \rangle - \langle s \nabla \varphi_{-1}, \phi \rangle = 0, \quad (5.112b)$$

$$\left\langle \frac{\rho(\varphi_{-1})}{\tau} s, \psi \right\rangle_{H^{-1}_{0,\sigma}, H^1_{0,\sigma}} - \langle \nabla s v, \psi \rangle_{H^{-1}_{0,\sigma}, H^1_{0,\sigma}}$$

$$+ (2\eta(\varphi_{-1})\varepsilon(s), \varepsilon(\psi)) - \langle r \nabla \varphi_{-1}, \psi \rangle_{H^{-1}_{0,\sigma}, H^1_{0,\sigma}} = 0, \quad (5.112c)$$

$$\langle -s, \psi \rangle_{H^{-1}_{0,\sigma}, H^1_{0,\sigma}} + \langle D_u \mathscr{J}[z_0], \psi \rangle_{H^{-1}_{0,\sigma}, H^1_{0,\sigma}} = 0, \quad (5.112d)$$

$$\lambda \in \left(T_{\mathbb{K}}(\varphi_0) \cap \{a_0^+\}^\perp \cap \{a_0^-\}^\perp \right)^0, \quad (5.112e)$$

$$s \in \left(\left[D\left(\left(T_{\mathbb{K}}(\varphi_0) \cap \{a_0^+\}^\perp \cap \{a_0^-\}^\perp \right)^0 \times H^1_{0,\sigma}(\Omega;\mathbb{R}^N) \right) \right]_2 \right)^0. \quad (5.112f)$$

Proof. Corollary 5.1.4 already ensures the existence of an adjoint state $(p, r, s) \in H^1(\Omega) \times H^1(\Omega) \times H^1_{0,\sigma}(\Omega;\mathbb{R}^N)$ and $\lambda \in H^1(\Omega)^*$ such that the system (5.112a)-(5.112d) is satisfied. It remains to show that (5.112e) and (5.112f) hold true.

By assumption u_0 is a minimizer of the following reduced optimal control problem

$$\min_{u \in L^2(\Omega;\mathbb{R}^N)} \overline{\mathscr{J}}(u), \quad (5.113)$$

where the objective functional $\overline{\mathscr{J}} : L^2(\Omega;\mathbb{R}^N) \to \mathbb{R}$ is defined by

$$\overline{\mathscr{J}}(u) := \mathscr{J}(\tilde{S}_{\overline{\Psi}}(u), u). \quad (5.114)$$

Consequently, the directional derivative of $\overline{\mathscr{J}}$ at u_0 is non-negative for every direction $h \in L^2(\Omega;\mathbb{R}^N)$, i.e.

$$D\overline{\mathscr{J}}[u_0](h) \geq 0, \ \forall h \in L^2(\Omega;\mathbb{R}^N). \quad (5.115)$$

Since u_0 is contained in $H^1_{0,\sigma}(\Omega;\mathbb{R}^N)$, due to Corollary 5.1.4, and $L^2(\Omega;\mathbb{R}^N)$ is dense in $H^1_{0,\sigma}(\Omega;\mathbb{R}^N)^*$, this yields

$$D\overline{\mathscr{J}}[u_0](h) \geq 0, \ \forall h \in H^1_{0,\sigma}(\Omega;\mathbb{R}^N)^*, \quad (5.116)$$

cf. e.g. [149, Lemma 3.1]. By the chain rule, this implies that for every $h \in H^1_{0,\sigma}(\Omega;\mathbb{R}^N)^*$ it holds that

$$0 \le \left\langle D_\varphi \mathscr{J}[z_0], D_\varphi \tilde{S}_{\overline{\Psi}}[u_0](h) \right\rangle + \langle D_u \mathscr{J}[z_0], h\rangle \tag{5.117}$$

$$= \left\langle D_\varphi \mathscr{J}[z_0], q \right\rangle + \langle D_u \mathscr{J}[z_0], h\rangle, \tag{5.118}$$

where q is determined by Theorem 5.1.2 via $(q,w,\zeta) = D\tilde{S}_{\overline{\Psi}}[u_0](h)$.

In order to show the inclusion (5.112f), we consider an arbitrary element (w^*,ζ^*) of the subsequent cone

$$(w^*,\zeta^*) \in \left(T_{\mathbb{K}}(\varphi_0) \cap \{a_0^+\}^\perp \cap \{a_0^-\}^\perp\right)^0 \times H^1_{0,\sigma}(\Omega;\mathbb{R}^N). \tag{5.119}$$

and define $h^* \in H^1_{0,\sigma}(\Omega;\mathbb{R}^N)^*$ by $h^* := [D(w^*,\zeta^*)]_2$, cf. (5.85), such that the following equation holds true

$$\begin{aligned} \langle h^*, \psi\rangle_{H^{-1}_{0,\sigma},H^1_{0,\sigma}} = &\left\langle \frac{\rho(\varphi_{-1})\zeta^*}{\tau}, \psi \right\rangle_{H^{-1}_{0,\sigma},H^1_{0,\sigma}} - (\zeta^* \otimes v, \nabla\psi) \\ &+ (2\eta(\varphi_{-1})\varepsilon(\zeta^*), \varepsilon(\psi)) - \langle w^*\nabla\varphi_{-1}, \psi\rangle_{H^{-1}_{0,\sigma},H^1_{0,\sigma}}. \end{aligned} \tag{5.120}$$

Due to Theorem 5.1.2 it holds that $(0,w^*,\zeta^*) = D\tilde{S}_{\overline{\Psi}}[u_0](h^*)$, since the following system is satisfied

$$\begin{aligned} 0 &\in T_{\mathbb{K}}(\varphi_0) \cap \{a_0^+\}^\perp \cap \{a_0^-\}^\perp, \\ \left\langle -w^*, \hat{\phi} \right\rangle &\ge 0,\ \forall \hat{\phi} \in T_{\mathbb{K}}(\varphi_0) \cap \{a_0^+\}^\perp \cap \{a_0^-\}^\perp, \\ \langle \zeta^*\nabla\varphi_{-1}, \phi\rangle &+ (m(\varphi_{-1})\nabla w^*, \nabla\phi) = 0, \\ \left\langle \frac{\rho(\varphi_{-1})\zeta^*}{\tau}, \psi \right\rangle_{H^{-1}_{0,\sigma},H^1_{0,\sigma}} &- (\zeta^* \otimes v, \nabla\psi) + (2\eta(\varphi_{-1})\varepsilon(\zeta^*), \varepsilon(\psi)) \\ &- \langle w^*\nabla\varphi_{-1}, \psi\rangle_{H^{-1}_{0,\sigma},H^1_{0,\sigma}} - \langle h^*, \psi\rangle_{H^{-1}_{0,\sigma},H^1_{0,\sigma}} = 0. \end{aligned}$$

Applying inequality (5.118) with respect to h^* leads to

$$0 \le \langle D_u \mathscr{J}[z_0], h^*\rangle = \langle s, h^*\rangle,$$

where we additionally used (5.112d). This concludes the proof of inclusion (5.112f).

To verify inclusion (5.112e) we consider an arbitrary element q^* of the critical cone, i.e. $q^* \in T_{\mathbb{K}}(\varphi_0) \cap \{a_0^+\}^\perp \cap \{a_0^-\}^\perp$. As above we define $h^* \in H^1_{0,\sigma}(\Omega;\mathbb{R}^N)^*$ and

$$(w^*,\zeta^*) := D^{-1}\left(-\frac{q^*}{\tau}, h^*\right) \in H^1(\Omega) \times H^1_{0,\sigma}(\Omega;\mathbb{R}^N) \tag{5.121}$$

such that the following system is satisfied for all $\phi \in H^1(\Omega)$ and $\psi \in H^1_{0,\sigma}(\Omega;\mathbb{R}^N)$

$$(\nabla q^*, \nabla\phi) - \langle w^*, \phi\rangle = 0, \tag{5.122}$$

$$\left\langle \frac{q^*}{\tau}, \phi \right\rangle + \langle \zeta^* \nabla\varphi_{-1}, \phi\rangle + (m(\varphi_{-1})\nabla w^*, \nabla\phi) = 0, \tag{5.123}$$

$$\begin{aligned}\left\langle \frac{\rho(\varphi_{-1})\zeta^*}{\tau}, \psi \right\rangle_{H^{-1}_{0,\sigma},H^1_{0,\sigma}} &- (\zeta^* \otimes \rho(\varphi_{-2})v_{-1}, \nabla\psi) \\ + \left(\zeta^* \otimes \frac{\rho_2-\rho_1}{2} m(\varphi_{-2})\nabla\mu_{-1}, \nabla\psi\right) &+ (2\eta(\varphi_{-1})\varepsilon(\zeta^*), \varepsilon(\psi)) \\ - \langle w^*\nabla\varphi_{-1}, \psi\rangle_{H^{-1}_{0,\sigma},H^1_{0,\sigma}} &- \langle h^*, \psi\rangle_{H^{-1}_{0,\sigma},H^1_{0,\sigma}} = 0,\end{aligned} \tag{5.124}$$

i.e. $(q^*, w^*, \zeta^*) = D\tilde{S}_{\overline{\Psi}}[u_0](h^*)$, cf. Theorem 5.1.2.

Then we apply (5.118) with respect to h^* to conclude

$$0 \le \left(D_\varphi \mathscr{J}[z_0], q^*\right) + \langle D_u \mathscr{J}[z_0], h^*\rangle \tag{5.125}$$

$$\begin{aligned}&= \left(D_\varphi \mathscr{J}[z_0], q^*\right) + \left\langle D_u \mathscr{J}[z_0], \frac{\rho(\varphi_{-1})\zeta^*}{\tau}\right\rangle \\ &\quad + \langle D_u \mathscr{J}[z_0], \operatorname{div}(\zeta^* \otimes v)\rangle \\ &\quad - \langle D_u \mathscr{J}[z_0], \operatorname{div}(2\eta(\varphi_{-1})\varepsilon(\zeta^*))\rangle \\ &\quad - \langle D_u \mathscr{J}[z_0], w^*\nabla\varphi_{-1}\rangle,\end{aligned} \tag{5.126}$$

where we additionally employed equation (5.124).

In combination with (5.112d) this yields

$$\begin{aligned}0 \le \left(D_\varphi \mathscr{J}[z_0], q^*\right) &+ \left\langle \frac{\rho(\varphi_{-1})\zeta^*}{\tau}, s\right\rangle_{H^{-1}_{0,\sigma},H^1_{0,\sigma}} - (\zeta^* \otimes v, \nabla s) \\ &+ (2\eta(\varphi_{-1})\varepsilon(\zeta^*), \varepsilon(s)) - \langle w^*\nabla\varphi_{-1}, s\rangle_{H^{-1}_{0,\sigma},H^1_{0,\sigma}}.\end{aligned} \tag{5.127}$$

With the help of (5.112c) this can be simplified to

$$0 \le \left(D_\varphi \mathscr{J}[z_0], q^*\right) + \langle r\nabla\varphi_{-1}, \zeta^*\rangle - \langle w^*\nabla\varphi_{-1}, s\rangle_{H^{-1}_{0,\sigma},H^1_{0,\sigma}} \tag{5.128}$$

$$= \left(D_\varphi \mathscr{J}[z_0], q^*\right) - \left\langle \frac{q^*}{\tau}, r\right\rangle - (m(\varphi_{-1})\nabla w^*, \nabla r) - \langle w^*\nabla\varphi_{-1}, s\rangle_{H^{-1}_{0,\sigma},H^1_{0,\sigma}}, \tag{5.129}$$

where we also used equation (5.123).

By applying (5.112b),(5.122) and (5.112a) (in this order) we further deduce

$$0 \le \left(D_\varphi \mathscr{J}[z_0], q^*\right) - \left\langle \frac{q^*}{\tau}, r \right\rangle - \langle p, w^* \rangle \tag{5.130}$$

$$= \left(D_\varphi \mathscr{J}[z_0], q^*\right) - \left\langle \frac{q^*}{\tau}, r \right\rangle - (\nabla p, \nabla q^*) \tag{5.131}$$

$$= - \langle \lambda, q^* \rangle, \tag{5.132}$$

Consequently, λ is an element of the polar cone $\left(T_{\mathbb{K}}(\varphi_0) \cap \{a_0^+\}^\perp \cap \{a_0^-\}^\perp\right)^0$, cf. Definition 1.3.2, which completes the proof of inclusion (5.112e). □

This concludes our analytical investigations of Section 5.1. In summary, we extended the results from the previous chapters to functions with arbitrary mean values and - more importantly - we established more restrictive stationarity conditions for the optimal control problem (I_Ψ). In combination with the results from Section 4.1, in particular Theorem 4.1.4, the system (5.112) constitutes a strong stationarity system for (I_Ψ), which is the most selective stationarity system available for (I_Ψ) up to this point.

5.2 A bundle-free implicit programming approach

We conclude our discussion of strong stationarity conditions for the optimal control of a semi-discrete Cahn-Hilliard-Navier-Stokes system with the presentation of an advanced numerical solver, which is specifically designed to target strong stationary points. For this purpose, we utilize a bundle-free implicit programming approach. In doing so, we take advantage of the characterization of the directional derivative of the control-to-state operator derived in the previous section.

Although similar solution methods are well established in finite dimensions, see e.g. [72, 142, 160, 172] and the references therein, the research on the application to infinite dimensional problems is more recent. However, in [115], the method has been successfully applied to a class of mathematical programs with equilibrium constraints, including a standard optimal control problem subject to a variational inequality in infinite dimensions.

Besides targeting strong stationary points, the subsequently developed solution algorithm further addresses another weakness of the solver presented in Section 4.3. In contrast to the regularizing Algorithm 3, which in most cases never computes a true feasible point of the optimal control problem (P_Ψ), the bundle-free approach computes feasible points of (P_Ψ) at every iteration.

Let us start by considering the reduced control problem introduced in Subsection 5.1.3

$$\min_{u\in L^2(\Omega;\mathbb{R}^N)^{M-1}} \overline{\mathscr{J}}(u) = \min_{u\in L^2(\Omega;\mathbb{R}^N)^{M-1}} \mathscr{J}(S_\Psi(u),u), \tag{5.133}$$

where $\mathscr{J}$ denotes the tracking type functional defined by (3.4) and S_Ψ represents the solution mapping (2.38).

We recall that every locally optimal point $\hat{u}$ of (5.133), with $S_\Psi(\hat{u}) = (\hat{\varphi},\hat{\mu},\hat{v})$ and the associated slack variable $\hat{a}$, is B-stationary, i.e. for every direction $h \in L^2(\Omega;\mathbb{R}^N)^{M-1}$ it holds that

$$\begin{aligned} 0 &\le D\overline{\mathscr{J}}[\hat{u}](h) && (5.134)\\ &= \left\langle D_\varphi \mathscr{J}[\hat{\varphi},\hat{\mu},\hat{v},\hat{u}], D_\varphi S_\Psi[\hat{u}](h)\right\rangle + \langle D_u \mathscr{J}[\hat{\varphi},\hat{\mu},\hat{v},\hat{u}],h\rangle && (5.135)\\ &= \left\langle \hat{\varphi}_{M-1} - \varphi_d, q_{M-1}\right\rangle + \xi\,\langle \hat{u},h\rangle, && (5.136)\end{aligned}$$

where we employed the directional derivative of $\mathscr{J}$ and the chain rule.

We will subsequently implement a numerical solution algorithm for the optimal control of the semi-discrete Cahn-Hilliard-Navier-Stokes system (2.38) with respect to the objective functional $\mathscr{J}$ given by (3.4). This facilitates a comparison of the solvers developed in Section 4.3 and Section 5.2.

In advance of our analytical results, the derivative of the corresponding control-to-state operator S_Ψ at the point $\hat{u}$ in direction h is represented by

$$(q,w,\zeta) = DS_\Psi[\hat{u}](h) = \left(D_\varphi S_\Psi[\hat{u}](h), D_\mu S_\Psi[\hat{u}](h), D_v S_\Psi[\hat{u}](h)\right), \tag{5.137}$$

where the triple $(q_{i+1}, w_{i+1}, \zeta_{i+1}) \in H^1(\Omega) \times H^1(\Omega) \times H^1_{0,\sigma}(\Omega;\mathbb{R}^N)$ satisfies the system

$$q_{i+1} \in T_{\mathbb{K}}(\hat{\varphi}_{i+1}) \cap \{\hat{a}^+_{i+1}\}^\perp \cap \{\hat{a}^-_{i+1}\}^\perp, \tag{5.138a}$$

$$\left\langle -\Delta q_{i+1} - w_{i+1} - \kappa q_i, \tilde{\phi} - q_{i+1} \right\rangle \geq 0, \forall \tilde{\phi} \in T_{\mathbb{K}}(\hat{\varphi}_{i+1}) \cap \{\hat{a}^+_{i+1}\}^\perp \cap \{\hat{a}^-_{i+1}\}^\perp, \tag{5.138b}$$

$$\begin{aligned} \frac{q_{i+1} - q_i}{\tau} + \zeta_{i+1} \nabla \hat{\varphi}_i + \hat{v}_{i+1} \nabla q_i - \operatorname{div}\left(m(\hat{\varphi}_i) \nabla w_{i+1}\right) \\ - \operatorname{div}\left(m'(\hat{\varphi}_i) q_i \nabla \hat{\mu}_{i+1}\right) = 0, \end{aligned} \tag{5.138c}$$

$$\begin{aligned} \frac{1}{\tau}(\rho'(\hat{\varphi}_i) q_i \hat{v}_{i+1} - \rho'(\hat{\varphi}_{i-1}) q_{i-1} \hat{v}_i) + \frac{1}{\tau}(\rho(\hat{\varphi}_i)\zeta_{i+1} - \rho(\hat{\varphi}_{i-1})\zeta_i) \\ + \operatorname{div}(\hat{v}_{i+1} \otimes (\rho'(\hat{\varphi}_{i-1}) q_{i-1} \hat{v}_i + \rho(\hat{\varphi}_{i-1})\zeta_i)) \\ - \operatorname{div}(\hat{v}_{i+1} \otimes (\frac{\rho_2 - \rho_1}{2} m'(\hat{\varphi}_{i-1}) q_{i-1} \nabla \hat{\mu}_i - \frac{\rho_2 - \rho_1}{2} m(\hat{\varphi}_{i-1}) \nabla w_i)) \\ + \operatorname{div}(\zeta_{i+1} \otimes (\rho(\hat{\varphi}_{i-1}) \hat{v}_i - \frac{\rho_2 - \rho_1}{2} m(\hat{\varphi}_{i-1}) \nabla \hat{\mu}_i)) - \hat{\mu}_{i+1} \nabla q_i \\ - w_{i+1} \nabla \hat{\varphi}_i - \operatorname{div}(2\eta'(\hat{\varphi}_i) q_i \varepsilon(\hat{v}_{i+1})) - \operatorname{div}(2\eta(\hat{\varphi}_i)\varepsilon(\zeta_{i+1})) - B h_{i+1} = 0, \end{aligned} \tag{5.138d}$$

for every $1 \leq i+1 \leq M-1$, cf. Theorem 5.1.2. Here, $B : U \to L^2(\Omega;\mathbb{R}^N)$ denotes the bounded linear operator introduced in Section 4.2.

Based on inequality (5.136) we verify that $\overline{h} = 0$ solves the following optimization problem

$$\begin{aligned} \min_{h \in L^2(\Omega;\mathbb{R}^N)^{M-1}} & \left\langle \hat{\varphi}_{M-1} - \varphi_d, q_{M-1} \right\rangle + \xi \left\langle \hat{u}, h \right\rangle \\ & \text{s.t. } DS_\Psi[\hat{u}](h) = (q, w, \zeta), \end{aligned} \tag{5.139}$$

if $\hat{u}$ is B-stationary. However, in general, i.e. for an arbitrary point $(\hat{\varphi}, \hat{\mu}, \hat{v}, \hat{u})$, the problem (5.139) need not have a solution. For this reason, we subsequently add a quadratic term to the objective in order to ensure the existence of solutions

$$\begin{aligned} \min_{h \in L^2(\Omega;\mathbb{R}^N)^{M-1}} & \mathscr{F}(h, q) := \left\langle \varphi_{M-1} - \varphi_d, q_{M-1} \right\rangle + \xi \left\langle u, h \right\rangle + \alpha \|h\|^2 \\ & \text{s.t. } DS_\Psi[u](h) = (q, w, \zeta). \end{aligned} \tag{5.140}$$

Here, α denotes an arbitrary positive constant. Clearly, any solution $\overline{h} \neq 0$ to (5.140) corresponds to a descent direction of $\overline{\mathscr{J}}$ at the point $\hat{u}$, since it holds that

$$D\overline{\mathscr{J}}[\hat{u}](\overline{h}) < D\overline{\mathscr{J}}[\hat{u}](\overline{h}) + \alpha \|\overline{h}\|^2 \leq D\overline{\mathscr{J}}[\hat{u}](0) = 0. \tag{5.141}$$

We summarize our observations in the following lemma, which is a direct consequence of the application of the theory developed in [115].

Lemma 5.2.1. *For an arbitrary point $u \in L^2(\Omega;\mathbb{R}^N)^{M-1}$ with $S(u) = (\varphi,\mu,v)$ and $\alpha > 0$ the following statements are satisfied.*

(I) The problem (5.140) *has a unique optimal solution $\overline{h} \in L^2(\Omega;\mathbb{R}^N)^{M-1}$.*

(II) If (φ,μ,v,u) is a locally optimal point of (P_Ψ), then $\overline{h} = 0$ is a solution to (5.140).

(III) If $\overline{h} \neq 0$ solves (5.140)*, then it is a descent direction for the reduced optimization problem* (5.133).

Proof. The existence of solutions to the problem (5.140) is verified by standard arguments from optimization theory. The remaining statements follow from [115, Lemma 2.1,Corollary 2.2 and Corollary 2.3], respectively. □

Motivated by the preceding lemma, we formulate the following conceptual algorithm.

Data: Initial data: $\varphi_{-1},\varphi_0,v_0,u^1,m,\eta,\tau,M,\varphi^d,\zeta,\alpha$ and $\varepsilon_{tol} > 0$

Set $k := 1$;

repeat

  Compute $(v^k,\varphi^k,\mu^k) = S(u^k)$ by solving the CHNS system (2.37);

  Calculate a descent direction h^k by solving the auxiliary problem (5.140);

  Find a step size τ^k and a new iterate $u^{k+1} := u^k + \tau^k h^k$ by performing an Armijo line search for the problem (5.133) at u^k along direction h^k;

  Set $k := k+1$;

until $\|h^k\| \leq \varepsilon_{tol}$;

Algorithm 5: conceptualAlgorithm

Due to the third property of Lemma 5.2.1, it is evident that the sequence $\{\overline{\mathscr{J}}(u^k)\}_{k\in\mathbb{N}}$ generated by Algorithm 5 is monotonically decreasing.

Moreover, [115, Theorem 2.5] ensures that the generated sequence $\{h^k\}_{k\in\mathbb{N}}$ of descent directions is converging to zero, if one of the following conditions is satisfied:

1. Either the sequence $\{\tau^k\}_{k\in\mathbb{N}}$ generated by the Armijo line search is bounded away from zero, i.e. $\exists_{\underline{\tau}>0}\forall_{k\in\mathbb{N}} \quad \tau^k \geq \underline{\tau}$,

2. or it holds that

$$\limsup_{k\to\infty} \frac{\overline{\mathscr{J}}(u^k + \overline{\tau}^k h^k) - \overline{\mathscr{J}}(u^k) - \overline{\tau}^k \overline{\mathscr{J}}'[u^k](h^k)}{\overline{\tau}^k} \leq 0, \tag{5.142}$$

where $\overline{\tau}^k > 0$ represents the smallest step size for which the line search still fails at step k.

For this reason, we add a 'robustification step' to Algorithm 5 in the subsequent section, in order to ensure that $\{\|h^k\|\}_{k\in\mathbb{N}}$ converges to zero. In the robustification step, the convergence rates of h^k and τ^k are compared and if the step size $\{\tau^k\}_{k\in\mathbb{N}}$ converges faster to zero than $\{\|h^k\|^2\}_{k\in\mathbb{N}}$, we execute one iteration of the regularizing Algorithm 3 to calculate an eligible control u^{k+1}.

5.2.1 Solving the primal and dual systems

In this section, we show in more detail how each of the steps of the conceptual algorithm is implemented.

A primal dual active set method

In order to compute a solution to the semi-discrete Cahn–Hilliard–Navier–Stokes system (2.37), i.e. to execute Line 3 of Algorithm 5, we utilize a primal dual active set method. For this purpose, we recall that the slack variable a_{i+1} is contained in $L^2(\Omega)$ and the variational inequality (2.37b) can be reformulated as a complementarity problem of the form (3.25). By inspection the complementarity system can be equivalently expressed as

$$-\Delta\varphi_{i+1} + a_{i+1} - \mu_{i+1} - \kappa\varphi_i = 0, \tag{5.143a}$$

$$\mathscr{C}(\varphi_{i+1}, a_{i+1}) = 0, \tag{5.143b}$$

where $\mathscr{C}$ denotes the following NCP-function

$$\mathscr{C}(\varphi, a) := a - \max(0, a + C(\varphi - 1)) + \max(0, -a - C(\varphi + 1)). \tag{5.144}$$

More precisely, (2.37b) implies (5.2.1) for every $C > 0$, and (5.2.1) for some $C > 0$ yields (2.37b). By Theorem 1.5.2 the NCP-function $\mathscr{C}$ is Newton differentiable from $L^p(\Omega)$ to $L^2(\Omega)$ for every $p > 2$, see also Definition 1.5.1.

For a given state

$$(v^k_{i+1}, \varphi^k_{i+1}, \mu^k_{i+1}, a^k_{i+1}) \in H^1(\Omega) \times H^1(\Omega) \times H^1_{0,\sigma}(\Omega;\mathbb{R}^N) \times L^2(\Omega)$$

we define the operative active and inactive sets as follows (with $C = 1$)

$$\mathscr{A}^1_k := \{\omega \in \Omega : a^k_{i+1} + (\varphi^k_{i+1} - 1) > 0\}, \tag{5.145a}$$

$$\mathscr{A}^{-1}_k := \{\omega \in \Omega : -a^k_{i+1} - (\varphi^k_{i+1} + 1) > 0\}, \tag{5.145b}$$

$$\mathscr{I}_k := \Omega \setminus (\mathscr{A}^1_k \cup \mathscr{A}^{-1}_k). \tag{5.145c}$$

Then the primal dual active set method for the semi-discrete Cahn–Hilliard–Navier–Stokes system consists in solving the system

$$\left\langle \frac{\varphi_{i+1}^{k+1} - \varphi_i}{\tau}, \phi \right\rangle + \left\langle v_{i+1}^{k+1} \nabla \varphi_i, \phi \right\rangle + \Big(m(\varphi_i) \nabla (\mu_{i+1})^{k+1}, \nabla \phi \Big) = 0, \tag{5.146a}$$

$$\Big(\nabla \varphi_{i+1}^{k+1}, \nabla \phi \Big) + \Big((a_{i+1})^{k+1}, \phi \Big) - \Big\langle (\mu_{i+1})^{k+1}, \phi \Big\rangle - \langle \kappa \varphi_i, \phi \rangle = 0, \tag{5.146b}$$

$$\begin{aligned} &\frac{1}{\tau} \left\langle \rho(\varphi_i) v_{i+1}^{k+1} - \rho(\varphi^{i-1}) v_i, \psi \right\rangle - \left(v_{i+1}^{k+1} \otimes \rho(\varphi_{i-1}) v_i, \nabla \psi \right) \\ &+ \left(v_{i+1}^{k+1} \otimes \frac{\rho_2 - \rho_1}{2} m(\varphi_{i-1}) \nabla \mu_i, \nabla \psi \right) + \Big(2\eta(\varphi_i) \varepsilon(v_{i+1}^{k+1}), \varepsilon(\psi) \Big) \\ &- \langle \mu_{i+1} \nabla \varphi_i, \psi \rangle_{H^{-1}, H_0^1} - \langle \operatorname{div} \psi, \xi_i \rangle - (B u_{i+1}, \psi) = 0, \end{aligned} \tag{5.146c}$$

$$-(\operatorname{div} v_{i+1}^{k+1}, \phi) = 0, \tag{5.146d}$$

in combination with

$$(\varphi_{i+1})^{k+1} = 1 \text{ on } \mathscr{A}_k^1, \quad (\varphi_{i+1})^{k+1} = -1 \text{ on } \mathscr{A}_k^{-1}, \tag{5.147a}$$

$$(a_{i+1})^{k+1} = 0 \text{ on } \mathscr{I}_k. \tag{5.147b}$$

to obtain the new iterate

$$(v_{i+1}^{k+1}, \varphi_{i+1}^{k+1}, \mu_{i+1}^{k+1}, a_{i+1}^{k+1}) \in H^1(\Omega) \times H^1(\Omega) \times H_{0,\sigma}^1(\Omega; \mathbb{R}^N) \times L^2(\Omega).$$

More precisely, we set up the following algorithm, which iterates over all time steps $i \in \{1, .., M-1\}$.

Data: Initial data: $\varphi_{-1}, \varphi_0, v_0, u, m, \eta, \tau, M, \varepsilon_2$

for $i = 0, \ldots, M-2$ **do**
  Set $k := 0$;
  $(\varphi_{i+1})^0 := \varphi_i$, $(\mu_{i+1})^0 := \mu_i$, $(v_{i+1})^0 := v_i$, $(a_{i+1})^0 := a_i$;
  repeat
    Determine the sets $\mathscr{A}_k^1, \mathscr{A}_k^{-1}, \mathscr{I}_k^1$ based on (5.145);
    Obtain $(v_{i+1}^{k+1}, \varphi_{i+1}^{k+1}, \mu_{i+1}^{k+1}, a_{i+1}^{k+1})$ by solving (5.146),(5.147);
    Set $k := k+1$;
  until $\|(v_{i+1}^{k+1} - v_{i+1}^k, \varphi_{i+1}^{k+1} - \varphi_{i+1}^k, \mu_{i+1}^{k+1} - \mu_{i+1}^k)\| < \varepsilon_2$;
end

Algorithm 6: Primal Dual Active Set method

The stopping criteria in line 8 is chosen based on the fact that the method can be shown to converge superlinearly in the fully discrete setting. The convergence of the primal dual active set method is thoroughly discussed e.g. in [109, 126]. In particular, [126, Proposition 4.1] establishes superlinear convergence for the primal dual active set method in the context of variational inequalities with bilateral constraints. The result is based on the connection of the primal dual active set method and certain semismooth Newton methods.

Determining a descent direction

The next challenge is to compute a suitable descent direction at the given point (φ, μ, v, u), which corresponds to Line 4 of Algorithm 5. We start by recalling that the tangent cone $T_{\mathbb{K}}(\varphi_{i+1})$ at the time step $i+1$ and the critical cone at φ_{i+1} can be written as follows

$$T_{\mathbb{K}}(\varphi_{i+1}) = \{\phi \in H^1(\Omega) | \phi \geq 0, \text{ q.e. on } \mathscr{A}_{\varphi_{i+1},1}, \phi \leq 0 \text{ q.e. on } \mathscr{A}_{\varphi_{i+1},2}\}, \tag{5.148}$$

$$\begin{aligned} T_{\mathbb{K}}(\varphi_{i+1}) \cap \{a_{i+1}^{+}\}^{\perp} \cap \{a_{i+1}^{-}\}^{\perp} = \{&\phi \in H^1(\Omega) | \phi \geq 0, \text{ q.e. on } \mathscr{A}_{\varphi_{i+1},1}, \\ &\phi \leq 0 \text{ q.e. on } \mathscr{A}_{\varphi_{i+1},2}, \phi = 0 \text{ a.e. on } \mathscr{A}^{+}_{\varphi_{i+1},1} \cup \mathscr{A}^{+}_{\varphi_{i+1},2}\}, \end{aligned} \tag{5.149}$$

cf. Definition 3.3.1. The abbreviation q.e. stands for quasi everywhere, which signifies that the relation holds up to a set of capacity zero, cf. e.g. [34]. For convenience, we briefly note that the capacity of a set $A \subset \Omega$ is defined as

$$\operatorname{cap}(A) := \inf\{\|\nabla\phi\|^2 \ : \ \phi \in H^1(\Omega), \phi \geq 1 \text{ a.e. in a neighborhood of } A\}. \tag{5.150}$$

A function $\phi : \Omega \to \mathbb{R}$ is called quasi-continuous if for all $\varepsilon > 0$, there exists an open set $O_\varepsilon \subset \Omega$, such that $\operatorname{cap}(O_\varepsilon) < \varepsilon$ and the function ϕ is continuous on $\Omega \setminus O_\varepsilon$. By [59, Theorem 6.1], every $\phi \in H^1(\Omega)$ possesses a quasi-continuous representative, which is uniquely determined up to a set of zero capacity. Further note that a set of zero capacity has measure zero, but the converse does not hold in general. For more information on capacity theory, we refer to e.g. [15, 34, 59].

In the following, we distinguish two cases. First, we consider the case, where the measure of the biactive sets is equal to zero, i.e.

$$m(\mathscr{A}^{0}_{\varphi_{i+1},1}) = m(\mathscr{A}^{0}_{\varphi_{i+1},2}) = 0. \tag{5.151}$$

Consequently, the active sets $\mathscr{A}_{\varphi_{i+1},1}, \mathscr{A}_{\varphi_{i+1},2}$ coincide with the strongly active sets $\mathscr{A}^{+}_{\varphi_{i+1},1}, \mathscr{A}^{+}_{\varphi_{i+1},2}$ up to a set of measure zero, which will be called strict complementarity.

In the second case, i.e. if $m(\mathscr{A}^0_{\varphi_{i+1},1}) + m(\mathscr{A}^0_{\varphi_{i+1},2}) > 0$, we say that strict complementarity fails.

Moreover, we assume that the active and biactive sets at each time step satisfy the following [109, Assumption (18)].

Assumption 5.2.1. *For $j \in \{1,2\}$ it holds that*

(I) $\mathscr{A}_{\varphi_{i+1},j} = \overline{\mathring{\mathscr{A}}_{\varphi_{i+1},j}}$;

(II) if $m(\mathscr{A}^0_{\varphi_{i+1},j}) = 0$, *then* $\operatorname{cap}(\mathscr{A}^0_{\varphi_{i+1},j}) = 0$ *or* $DS_\Psi[u](h) = (q,w,\zeta)$ *with*

$$q_{i+1} = 0 \text{ q.e. on } \mathscr{A}_{\varphi_{i+1},j}; \tag{5.152}$$

(III) if $m(\mathscr{A}^0_{\varphi_{i+1},j}) > 0$, *then there exist* $\tilde{\varepsilon} > 0$ *and* $\tilde{\gamma} > 0$ *such that for every* $\forall \gamma > \tilde{\gamma}$ *it holds that*

$$q^\gamma_{i+1} \geq 0 \text{ a.e. on } \{\omega \in \Omega \mid \operatorname{dist}(\omega, \mathscr{A}_{\varphi_{i+1},j}) < \tilde{\varepsilon}\} \setminus \mathscr{A}_{\varphi_{i+1},j}. \tag{5.153}$$

Here, q^γ_{i+1} *corresponds to the solution of the system* (5.138c), (5.138d), (5.161) *introduced below, where we also discuss condition (III) in more detail.*

The assumption excludes some exceptional shapes of the active and biactive sets and condition (*II*) ensures that the variational inequality (5.138a),(5.138b), which characterizes the directional derivative, can be equivalently rewritten as

$$q_{i+1} = 0, \text{ q.e. on } \mathscr{A}_{\varphi_{i+1},1} \cup \mathscr{A}_{\varphi_{i+1},2}, \tag{5.154a}$$

$$\langle -\Delta q_{i+1} - w_{i+1} - \kappa q_i, \phi \rangle = 0, \ \forall \phi \in H^1(\Omega) : \phi = 0 \text{ q.e. } \mathscr{A}_{\varphi_{i+1},1} \cup \mathscr{A}_{\varphi_{i+1},2}, \tag{5.154b}$$

if strict complementarity holds. Since φ_{i+1} is continuous, the inactive set $\mathscr{I}_{\varphi_{i+1}}$ is open and (5.154) can be reformulated as

$$q_{i+1} \in H^1(\mathscr{I}_{\varphi_{i+1}}), \tag{5.155a}$$

$$\langle -\Delta q_{i+1} - w_{i+1} - \kappa q_i, \phi \rangle = 0, \ \forall \phi \in H^1(\mathscr{I}_{\varphi_{i+1}}), \tag{5.155b}$$

cf. e.g. [95]. As a consequence, the optimization problem (5.140) is an infinite-dimensional quadratic program. Thus, the well-known Zowe-Kurcyusz theorem ensures the existence of an adjoint state

$$(p,r,s) \in H^1(\Omega)^M \times H^1(\Omega)^M \times H^1_{0,\sigma}(\Omega;\mathbb{R}^N)^{M-1} \tag{5.156}$$

such that the subsequent adjoint system is fulfilled

$$r_{i-1} \in H^1(\mathscr{I}_{\varphi_i}) \tag{5.157a}$$

$$\begin{aligned}
-\frac{1}{\tau}(p_i - p_{i-1}) + m'(\varphi_i)\nabla\mu_{i+1}\nabla p_i - \operatorname{div}(p_i v_{i+1}) - \Delta r_{i-1}& \\
-\kappa r_{i+1} - \frac{1}{\tau}\rho'(\varphi_i)v_{i+1}\cdot(s_{i+1}-s_i)& \\
-(\rho'(\varphi_i)v_{i+1} - \frac{\rho_2-\rho_1}{2}m'(\varphi_i)\nabla\mu_{i+1})(Ds_{i+1})^\top v_{i+2}& \\
+2\eta'(\varphi_i)\varepsilon(v_{i+1}) : Ds_i + \operatorname{div}(\mu_{i+1}s_i) - i_{M-1}(i)(\varphi_i - \varphi_d)_{|H^1(\mathscr{I}_{\varphi_i})} &= 0,
\end{aligned} \tag{5.157b}$$

$$\begin{aligned}
-r_{i-1} - \operatorname{div}(m(\varphi_{i-1})\nabla p_{i-1}) - \operatorname{div}(\frac{\rho_2-\rho_1}{2}m(\varphi_{i-1})(Ds_i)^\top v_{i+1})& \\
-s_{i-1}\cdot\nabla\varphi_{i-1} &= 0,
\end{aligned} \tag{5.157c}$$

$$\begin{aligned}
-\frac{1}{\tau}\rho(\varphi_{j-1})(s_j - s_{j-1}) - \rho(\varphi_{j-1})(Ds_j)^\top v_{j+1}& \\
-(Ds_{j-1})(\rho(\varphi_{j-2})v_{j-1} - \frac{\rho_2-\rho_1}{2}m(\varphi_{j-2})\nabla\mu_{j-1})& \\
-\operatorname{div}(2\eta(\varphi_{j-1})\varepsilon(s_{j-1})) + p_{j-1}\nabla\varphi_{j-1} &= 0,
\end{aligned} \tag{5.157d}$$

$$\nu u_i + \alpha h_i - B^* s_i = 0. \tag{5.157e}$$

cf. e.g. Subsection 4.1.1 and [191]. The system (5.157) can be solved by a standard Newton method to obtain an appropriate descent direction $h \in L^2(\Omega;\mathbb{R}^N)^{M-1}$.

If strict complementarity fails, we resort to a regularization method. More precisely, we exploit the fact that it is not necessary to solve the problem (5.140) exactly in order to obtain a descent direction for $\overline{\mathscr{J}}$. Instead, it can be guaranteed that the solutions of certain regularized problems still constitute a descent direction for $\overline{\mathscr{J}}$ as long as the approximation is close enough.

Based on the characterization (5.149), we define the penalization $\tilde{\Psi}_\varepsilon : L^2(\Omega) \to \mathbb{R}$ of the indicator function $i_{T_{\mathbb{K}}(\varphi_{i+1})\cap\{a_{i+1}^+\}^\perp\cap\{a_{i+1}^-\}^\perp}$ of the critical cone by

$$\begin{aligned}
\tilde{\Psi}_\varepsilon(q_{i+1}) :=& \frac{1}{2}\|\chi_{\mathscr{A}^+_{\varphi_{i+1},1}\cup\mathscr{A}^+_{\varphi_{i+1},2}} q_{i+1}\|^2 + \int_\Omega \chi_{\mathscr{A}_{\varphi_{i+1},1}} \max\nolimits_\varepsilon(0,-q_{i+1})dx \\
&+ \int_\Omega \chi_{\mathscr{A}_{\varphi_{i+1},2}} \max\nolimits_\varepsilon(0,q_{i+1})dx,
\end{aligned} \tag{5.158}$$

where $\varepsilon > 0$ is arbitrarily fixed, $\chi_{\mathscr{A}}$ represents the characteristic function of $\mathscr{A}$, and $\max_\varepsilon$ with $\varepsilon > 0$ denotes a C^2-smoothing of the max-operator given by

$$\max_\varepsilon(0,\varphi) := \begin{cases} \varphi - \frac{\varepsilon}{2} & \text{if } \varphi \geq \varepsilon \\ \frac{\varphi^3}{\varepsilon^2} - \frac{\varphi^4}{2\varepsilon^3} & \text{if } 0 < \varphi < \varepsilon \\ 0 & \text{if } \varphi \leq 0 \end{cases}. \tag{5.159}$$

Then the variational inequality (5.138a),(5.138b) is replaced by the following penalized equation

$$-\Delta q_{i+1} - w_{i+1} - \kappa q_i + \gamma\,\tilde{\Psi}_\varepsilon{}'(q_{i+1}) = 0, \tag{5.160}$$

which is equivalent to

$$\begin{aligned} &-\Delta q_{i+1} - w_{i+1} - \kappa q_i + \gamma\chi_{\mathscr{A}^+_{\varphi_{i+1},1}\cup\mathscr{A}^+_{\varphi_{i+1},2}} q_{i+1} \\ &-\gamma\chi_{\mathscr{A}_{\varphi_{i+1},1}} \max{}'_\varepsilon(0,-q_{i+1}) + \gamma\chi_{\mathscr{A}_{\varphi_{i+1},2}} \max{}'_\varepsilon(0,q_{i+1}) = 0. \end{aligned} \tag{5.161}$$

Here, $\gamma > 0$ represents the corresponding penalty parameter. This allows us to formulate the following regularized auxiliary program

$$\begin{aligned} &\min_{h\in L^2(\Omega;\mathbb{R}^N)^{M-1}} \mathscr{F}(h,q) = \left\langle \hat{\varphi}_{M-1} - \varphi_d, q_{M-1}\right\rangle + \xi\,\langle \hat{u}, h\rangle + \alpha\|h\|^2 \\ &\text{s.t. } \forall_{i\in\{1,..,M-1\}}(q_{i+1}, w_{i+1}, \zeta_{i+1}) \text{ solves (5.138c), (5.138d), (5.161)} \end{aligned} \tag{5.162}$$

We point out that the penalization is applied directly to the lower-level problem of the auxiliary program (5.140), which characterizes the descent directions of $\overline{\mathscr{J}}$.

The subsequent corollary establishes the existence of solutions to the penalized system (5.138c), (5.138d), (5.161) and verifies that the penalization is consistent in the sense specified in the second assertion.

Corollary 5.2.1. *Let $\varepsilon > 0$, $h \in L^2(\Omega;\mathbb{R}^N)^{M-1}$ be given and let $(\hat{\varphi}, \hat{\mu}, \hat{v}, \hat{u})$ be an arbitrary solution of the semi-discrete Cahn–Hilliard–Navier–Stokes system* (2.37)*.*

1. *For every $\gamma > 0$ the associated regularized system* (5.138c)*,* (5.138d)*,* (5.161) *possesses a solution for all $i = 0,...,M-1$.*

2. *Let further $\{\gamma^k\}_{k\in\mathbb{N}}$ be a given sequence with $\gamma^k \to \infty$ and let*

$$(q^{(k)}, w^{(k)}, \zeta^{(k)}) \in H^1(\Omega)^M \times H^1(\Omega)^M \times H^1_{0,\sigma}(\Omega;\mathbb{R}^N)^{M-1} \tag{5.163}$$

be a corresponding sequence of solutions to the associated systems (5.138c)*,* (5.138d)*,* (5.161)*.*

Then there exists a subsequence denoted by $\left\{(q^{(m)}, w^{(m)}, \zeta^{(m)})\right\}_{m\in\mathbb{N}}$ *and an element* (q,w,ζ) *such that*

$$q^{(m)} \rightharpoonup q \text{ in } H^1(\Omega)^M, \quad w^{(m)} \rightharpoonup w \text{ in } H^1(\Omega)^{M-1}, \tag{5.164a}$$

$$\zeta^{(m)} \rightharpoonup \zeta \text{ in } H^1_{0,\sigma}(\Omega;\mathbb{R}^N)^{M-1}, \tag{5.164b}$$

and (q,w,ζ) *satisfies the system* (5.138).

Proof. First, we observe that the system (5.138c), (5.138d), (5.161) can be rewritten as a generalized Cahn-Hilliard-Navier-Stokes system, which was defined in Definition 2.2.2, as follows

$$-\Delta q_{i+1} - w_{i+1} + \gamma\, \tilde{\Psi}_\varepsilon{}'(q_{i+1}) = \Theta^{(n)}_{1,i}, \tag{5.165a}$$

$$\frac{q_{i+1}-q_i}{\tau} + \zeta_{i+1}\nabla\hat{\varphi}_i - \operatorname{div}\left(m(\hat{\varphi}_i)\nabla w_{i+1}\right) = \Theta^{(n)}_{2,i} \tag{5.165b}$$

$$\begin{aligned}
&\frac{1}{\tau}(\rho(\hat{\varphi}_i)\zeta_{i+1} - \rho(\hat{\varphi}_{i-1})\zeta_i)\\
&+\operatorname{div}(\zeta_{i+1}\otimes(\rho(\hat{\varphi}_{i-1})\hat{v}_i - \frac{\rho_2-\rho_1}{2}m(\hat{\varphi}_{i-1})\nabla\hat{\mu}_i))\\
&-\operatorname{div}(2\eta(\hat{\varphi}_i)\varepsilon(\zeta_{i+1})) - w_{i+1}\nabla\hat{\varphi}_i - Bh_{i+1} = \Theta^{(n)}_{3,i}.
\end{aligned} \tag{5.165c}$$

Here the functionals $\Theta^{(n)}_{1,i}, \Theta^{(n)}_{2,i}$ and $\Theta^{(n)}_{3,i}$ are given by

$$\Theta^{(n)}_{1,i} = \kappa q_i, \tag{5.166}$$

$$\Theta^{(n)}_{2,i} = -\hat{v}_{i+1}\nabla q_i + \operatorname{div}\left(m'(\hat{\varphi}_i)q_i\nabla\hat{\mu}_{i+1}\right), \tag{5.167}$$

$$\begin{aligned}
\Theta^{(n)}_{3,i} = &-\frac{1}{\tau}(\rho'(\hat{\varphi}_i)q_i\hat{v}_{i+1} - \rho'(\hat{\varphi}_{i-1})q_{i-1}\hat{v}_i)\\
&-\operatorname{div}(\hat{v}_{i+1}\otimes(\rho'(\hat{\varphi}_{i-1})q_{i-1}\hat{v}_i + \rho(\hat{\varphi}_{i-1})\zeta_i))\\
&+\operatorname{div}(\hat{v}_{i+1}\otimes(\frac{\rho_2-\rho_1}{2}m'(\hat{\varphi}_{i-1})q_{i-1}\nabla\hat{\mu}_i - \frac{\rho_2-\rho_1}{2}m(\hat{\varphi}_{i-1})\nabla w_i))\\
&+\operatorname{div}(2\eta'(\hat{\varphi}_i)q_i\varepsilon(\hat{v}_{i+1})) + \hat{\mu}_{i+1}\nabla q_i,
\end{aligned} \tag{5.168}$$

and only contain the unknown quantities of the previous time steps.

Thus the assertions from Corollary 5.2.1 follow directly from the theory developed in Chapter 2 and Section 4.1. More precisely, the existence and the boundedness of solutions follows by induction over the time step $i = 0,..,M-1$ at the hands of Theorem 2.2.1 and Lemma 2.2.2, analogously to the proof of Theorem 2.2.2 and Lemma 2.2.4, respectively. We point out that the system (5.138c), (5.138d), (5.161) satisfies Assumption (2.50), since $(\hat{\varphi}, \hat{\mu}, \hat{v}, \hat{u})$ solves the semi-discrete Cahn–Hilliard–Navier–Stokes system (2.37) and, in particular, equation (2.37a).

The second assertion follows by the same convergence arguments as applied, e.g., in Theorem 3.2.1 and Theorem 4.1.1. Since the solutions are bounded by an energy-type estimate, cf. Lemma (2.2.1), there exists a weakly convergent subsequence $\left\{(q^{(m)}, w^{(m)}, \zeta^{(m)})\right\}_{m\in\mathbb{N}}$ and a point (q,w,ζ) such that (5.164) is satisfied. Analogously to the proof of Theorem 4.1.1, it is shown that the limit point (q,w,ζ) solves the system (5.138). In this process, Assumption 5.2.1*(III)* ensures that the penalization operator $\tilde{\Psi}_\varepsilon$ approximates $i_{T_{\mathbb{K}}(\varphi_{i+1})\cap\{a^+_{i+1}\}^\perp\cap\{a^-_{i+1}\}^\perp}$ in the sense of Assumption 4.1.1*(II)*, cf. also [109]. □

In order to take a closer look at the properties of the solutions to (5.162), we fix $\varepsilon > 0$ and $\gamma > 0$ and consider an arbitrarily fixed solution $(\hat{\varphi}, \hat{\mu}, \hat{v}, \hat{u})$ of the primal system (2.37) along with a given direction $h \in L^2(\Omega;\mathbb{R}^N)^{M-1}$. Moreover, let (q,w,ζ) denote the solution of the associated system (5.138), whereas $(q^{\varepsilon,\gamma}, w^{\varepsilon,\gamma}, \zeta^{\varepsilon,\gamma})$ represents the corresponding solution to the regularized system (5.138c), (5.138d), (5.161).

Then it holds that

$$
\begin{aligned}
D\overline{\mathscr{J}}[\hat{u}](h) &= \left\langle \hat{\varphi}_{M-1} - \varphi_d, q_{M-1}\right\rangle + \xi \left\langle \hat{u}, h\right\rangle, && (5.169)\\
&= \left\langle \hat{\varphi}_{M-1} - \varphi_d, q^{\varepsilon,\gamma}_{M-1}\right\rangle + \xi \left\langle \hat{u}, h\right\rangle + \left\langle \hat{\varphi}_{M-1} - \varphi_d, q - q^{\varepsilon,\gamma}_{M-1}\right\rangle, && (5.170)\\
&= \mathscr{F}(h, q^{\varepsilon,\gamma}) + \left(\left\langle \hat{\varphi}_{M-1} - \varphi_d, q - q^{\varepsilon,\gamma}_{M-1}\right\rangle - \alpha\|h\|^2\right). && (5.171)
\end{aligned}
$$

Thus, since $q^{\varepsilon,\gamma}$ converges weakly to q for $\gamma \to \infty$ in $H^1(\Omega)^M$ due to Corollary 5.2.1, the derivative of $\overline{\mathscr{J}}$ in direction h can be bounded by $\mathscr{F}(h, q^{\varepsilon,\gamma})$ if γ is sufficiently large. This leads to the following proposition.

Proposition 5.2.1. *Let* $\varepsilon > 0$ *be given and let* $(\hat{\varphi}, \hat{\mu}, \hat{v}, \hat{u})$ *be a solution of* (2.37). *For a given sequence* $\{\gamma^k\}_{k\in\mathbb{N}}$ *with* $\gamma^k \to \infty$ *let* $h^k \in L^2(\Omega;\mathbb{R}^N)^{M-1}$ *with*

$$
(q^{\varepsilon,k}, w^{\varepsilon,k}, \zeta^{\varepsilon,k}) \in H^1(\Omega)^M \times H^1(\Omega)^M \times H^1_{0,\sigma}(\Omega;\mathbb{R}^N)^{M-1} \qquad (5.172)
$$

be the solution of the corresponding auxiliary problem (5.162) *such that*

$$
\liminf_{k\to\infty} \|h^k\| > 0. \qquad (5.173)
$$

Then there exists $\overline{k} \in \mathbb{N}$ *such that* $h_{\overline{k}}$ *is a descent direction for* $\overline{\mathscr{J}}$ *at* $\hat{u}$.

Proof. Since h^k is bounded in $L^2(\Omega;\mathbb{R}^N)^{M-1}$, the second assertion of Corollary 5.2.1 ensures the existence of a $\overline{k} \in \mathbb{N}$ such that

$$
\left\langle \hat{\varphi}_{M-1} - \varphi_d, q - q^{\varepsilon,\overline{k}}_{M-1}\right\rangle < \alpha\|h_{\overline{k}}\|^2. \qquad (5.174)
$$

In combination with equation (5.171), this yields

$$D\overline{\mathscr{J}}[\hat{u}](h_{\bar{k}}) < \mathscr{F}(h_{\bar{k}}, q^{\varepsilon,\bar{k}}) \leq \mathscr{F}(0,0) = 0, \tag{5.175}$$

where the last inequality follows from the fact that $h_{\bar{k}}$ solves the problem (5.162). $\square$

Remark 5.2.1. *From the proof of Proposition 5.2.1, in particular, inequality* (5.175)*, it is evident that if there exists a $C > 0$ such that, for every $k \in \mathbb{N}$, it holds that $\mathscr{F}(h_k, q^{\varepsilon,k}) \leq -C$, then it can be additionally concluded that*

$$D\overline{\mathscr{J}}[\hat{u}](h_{\bar{k}}) \leq -C. \tag{5.176}$$

The preceding proposition ensures that a solution of the regularized programs (5.162) constitutes a descent direction for $\overline{\mathscr{J}}$ at $\hat{u}$ as long as inequality (5.174) is satisfied. The existence of such a solution is verified by standard optimization methods.

Corollary 5.2.2. *For every $\gamma > 0$ and $\varepsilon > 0$ the regularized problem* (5.162) *possesses a global solution.*

Proof. Since the objective functional is convex, weakly lower-semicontinuous, bounded from below and partially coercive with respect to h, cf. Assumption 3.1.1, we proceed analogously to the proof of Theorem 3.2.1 to ensure the existence of global solutions. $\square$

Due to the Fréchet differentiability of the associated constraint mapping, [191, Theorem 4.1] is employed once more to derive necessary first-order optimality conditions, which characterize a locally optimal point of (5.162).

Corollary 5.2.3. *For given $\gamma, \varepsilon > 0$ let $h \in L^2(\Omega;\mathbb{R}^N)^{M-1}$ be a minimizer of* (5.162) *with $(q,w,\zeta) \in H^1(\Omega)^M \times H^1(\Omega)^M \times H^1_{0,\sigma}(\Omega;\mathbb{R}^N)^{M-1}$.*

Then there exist adjoint states

$$(p,r,s) \in L^2(\Omega)^M \times L^2(\Omega)^M \times H^1_{0,\sigma}(\Omega;\mathbb{R}^N)^{M-1} \tag{5.177}$$

such that

$$
\begin{aligned}
-\frac{1}{\tau}(p_i - p_{i-1}) + m'(\varphi_i)\nabla\mu_{i+1}\nabla p_i - \operatorname{div}(p_i v_{i+1}) - \Delta r_{i-1} \\
+\gamma\tilde{\Psi}''_\varepsilon(q_i)^* r_{i-1} - \kappa r_{i+1} - \frac{1}{\tau}\rho'(\varphi_i) v_{i+1}\cdot(s_{i+1} - s_i) \\
-(\rho'(\varphi_i)v_{i+1} - \frac{\rho_2 - \rho_1}{2} m'(\varphi_i)\nabla\mu_{i+1})(Ds_{i+1})^\top v_{i+2} \\
+2\eta'(\varphi_i)\varepsilon(v_{i+1}) : Ds_i + \operatorname{div}(\mu_{i+1}s_i) - \chi_{M-1}(i)(\varphi_i - \varphi_d) &= 0, \quad (5.178a)\\
-r_{i-1} - \operatorname{div}(m(\varphi_{i-1})\nabla p_{i-1}) - \operatorname{div}(\frac{\rho_2 - \rho_1}{2} m(\varphi_{i-1})(Ds_i)^\top v_{i+1}) \\
-s_{i-1}\cdot\nabla\varphi_{i-1} &= 0, \quad (5.178b)\\
-\frac{1}{\tau}\rho(\varphi_{j-1})(s_j - s_{j-1}) - \rho(\varphi_{j-1})(Ds_j)^\top v_{j+1} \\
-(Ds_{j-1})(\rho(\varphi_{j-2})v_{j-1} - \frac{\rho_2 - \rho_1}{2} m(\varphi_{j-2})\nabla\mu_{j-1}) \\
-\operatorname{div}(2\eta(\varphi_{j-1})\varepsilon(s_{j-1})) + p_{j-1}\nabla\varphi_{j-1} &= 0, \quad (5.178c)\\
\nu u_i + \alpha h_i - B^* s_i &= 0, \quad (5.178d)
\end{aligned}
$$

where χ_{M-1} denotes the characteristic function of $M-1$ defined in Section 1.1.

Proof. It is sufficient to note that the penalty function $\tilde{\Psi}_\varepsilon : L^2(\Omega) \to \mathbb{R}$ is twice continuously Fréchet differentiable and the second derivative at a point $q \in L^2(\Omega)$ in direction $h \in L^2(\Omega)$ is given by

$$
\tilde{\Psi}_\varepsilon{}''[q](h) = \chi_{\mathscr{A}^+_{\varphi_{i+1},1} \cup \mathscr{A}^+_{\varphi_{i+1},2}} h + \chi_{\mathscr{A}_{\varphi_{i+1},1}} \max{}''_\varepsilon(0,-q)h + \chi_{\mathscr{A}_{\varphi_{i+1},2}} \max{}''_\varepsilon(0,q)h \quad (5.179)
$$

where the product of $\max''_\varepsilon(0,q)$ and h is formed pointwise almost everywhere. Then the rest of the proof is analogous to the proof of Theorem 4.1.2. □

Following Proposition 5.2.1 and Corollary 5.2.3, we formulate Algorithm 7 to compute a descent direction for $\overline{\mathscr{J}}$ at $\hat{u}$

Data: $\hat{\varphi}, \hat{\mu}, \hat{v}, \hat{u}, m, \eta, \tau, M$; φ^d, ζ; $\alpha, \gamma_0, \varepsilon$
Set $(r^M, p^M, s^M) := (0,0,0)$;
for $i = M, \ldots, 1$ **do**
  Determine the sets $\mathscr{A}^0_{\varphi_{i-1},1}, \mathscr{A}^0_{\varphi_{i-1},2}$ via (3.20),(3.21);
  if $m(\mathscr{A}^0_{\varphi_{i-1},1}) = m(\mathscr{A}^0_{\varphi_{i-1},2}) = 0$ **then**
    Solve the system (5.157) to compute $(r^{i-1}, p^{i-1}, s^{i-1})$;
  end
  else
    Set $\gamma := \gamma_0$;
    repeat
      Increase γ;
      Solve the system (5.178) to compute $(r^{i-1}, p^{i-1}, s^{i-1})$;
    until (5.174) *holds true*;
  end
  Set $h_{i-1} := \frac{1}{\alpha}(B^* s_{i-1} - \nu u_{i-1})$;
end

Algorithm 7: Computation of descent direction

A standard Newton method is used to solve the systems of partial differential equations (5.157) and (5.178).

As mentioned above, we further supplement Algorithm 5 with a robustification step, which compares the convergence rates of the the descent direction and the step sizes. More precisely, we add a counter σ, which is incrementally increased if it holds that

$$\tau^k < C_\sigma \|h^k\|^2. \tag{5.180}$$

If it reaches a certain threshold σ_{max}, we resort to Algorithm 3 in order to compute the next iterate u^{k+1}. This allows us to guarantee the convergence of the descent directions $\{h^k\}_{k\in\mathbb{N}}$ while still targeting strong stationary points.

In summary, we developed the following Algorithm 8 for solving the optimal control problem.

Similar to Section 4.2, we employ the finite element method and discretize the primal and dual systems using the Taylor-Hood elements based on the finite dimensional spaces V_1^i and V_2^i defined in (4.92)-(4.94). For the corresponding notation and further details we refer to Subsection 4.2.1, where it is properly introduced.

As noted in Section 4.2, it is highly recommended to reduce the computational cost of solving these large-scale systems by incorporating an appropriate mesh adaptation process. For this purpose, we rely on the dual weighted residual-based

Data: $\varphi_{-1}, \varphi_0, v_0, u_1, m, \eta, \tau, M$; φ^d, ζ; $\alpha, \gamma_0, C_\sigma, \sigma_{max}$; $\varepsilon_2, \varepsilon_{tol}$;

Set $k := 1$ and $\sigma := 0$;
repeat
  for $i = 0, \ldots, M$ **do**
    Set $j := 0$;
    $\varphi_{i+1}^0 := \varphi_i$, $\mu_{i+1}^0 := \mu_i$, $v_{i+1}^0 := v_i$, $a_{i+1}^0 := a_i$;
    repeat
      Determine the sets $\mathscr{A}_j^1, \mathscr{A}_j^{-1}, \mathscr{I}_j^1$ based on (5.145);
      Obtain $(v_{i+1}^{j+1}, \varphi_{i+1}^{j+1}, \mu_{i+1}^{j+1}, a_{i+1}^{j+1})$ by solving (5.146)-(5.147);
      Set $j := j + 1$;
    until $\|(v_{i+1}^{j+1} - v_{i+1}^j, \varphi_{i+1}^{j+1} - \varphi_{i+1}^j, \mu_{i+1}^{j+1} - \mu_{i+1}^j)\| < \varepsilon_2$;
  end
  Set $(r^M, p^M, s^M) := (0, 0, 0)$;
  for $i = M, \ldots, 1$ **do**
    Determine the sets $\mathscr{A}_{\varphi_{i-1},1}^0, \mathscr{A}_{\varphi_{i-1},2}^0$ via (3.20),(3.21);
    if $m(\mathscr{A}_{\varphi_{i-1},1}^0) = m(\mathscr{A}_{\varphi_{i-1},2}^0) = 0$ **then**
      Solve the system (5.157) to compute $(r^{i-1}, p^{i-1}, s^{i-1})$;
    end
    else
      Set $\gamma = \gamma_0$;
      repeat
        Increase γ ;
        Solve the system (5.178) to compute $(r^{i-1}, p^{i-1}, s^{i-1})$;
      until (5.174) *holds true*;
    end
    Set $h_{i-1} := \frac{1}{\alpha}(B^* s_{i-1} - \nu u_{i-1})$;
  end
  Find a step size τ^k and a new iterate $u^{k+1} := u^k + \tau^k h^k$ by performing a Armijo line search for the problem (5.133) at u^k along direction h^k;
  if (5.180) *fails* **then**
    $\sigma := \sigma + 1$;
  end
  if $\sigma > \sigma_{max}$ **then**
    Set $k := k + 1$ and $\sigma := 0$;
    Compute u_{k+1} by executing Line 3 to Line 11 of Algorithm 3;
  end
until $\|h^k\| \le \varepsilon_{tol}$;

Algorithm 8: Solution Algorithm

a posteriori error estimator developed in Section 4.2 and supplement Algorithm 8 with the subsequent mesh adaptation loop.

Data: Initial data: $\theta_r, \theta_c, \Xi_{\max}$

repeat

  Compute a solution on the current mesh via Algorithm 8;

  Calculate the error indicators via (4.145);

  Identify the sets $\mathscr{M}_r, \mathscr{M}_c$ of cells to refine/coarsen based on (4.146)/(4.147);

  Adapt $(\mathscr{T}^i)_{i=0}^{M-1}$ based on $\mathscr{M}_r$ and $\mathscr{M}_c$;

until $\sum_{i=0}^{M-1} |\mathscr{T}^i| < \Xi_{\max}$;

Algorithm 9: Mesh adaptation process

5.2.2 Numerical results

Finally, we illustrate the performance of the proposed Algorithm 8 for solving the optimization problem (5.133). For this purpose, we come back to the two examples from Section 4.3.1 in order to facilitate a comparison of the two algorithms.

As before, the implementation is done in C++ with the help of the finite element toolbox FEniCS [140], the PETSc linear algebra backend [17], and the linear solver MUMPS [13]. The algorithm for the line search in line 27 is taken from the GNU scientific library [1]. Moreover, we utilize the toolbox ALBERTA [171] to generate, store and adapt the spatial meshes.

The parameters for fluid behavior and the marking process are extracted from Section 4.3.1. We briefly recite them here for the convenience of the reader. The fluid densities are given by $\rho_1 = 1000$, $\rho_2 = 100$. The viscosities are set to $\eta_1 = 10$, $\eta_2 = 1$, and the mobility is $m(\varphi) \equiv \frac{1}{12500}$. We use $\varepsilon = 0.04$ and $\sigma = 24.5 \cdot \frac{2}{\pi}$. The time horizon is set to $T = 1.0$ and the time step size is $\tau = 0.00125$.

For the marking procedure we use the parameters $\theta^r = 0.7$ and $\theta^c = 0.01$. The mesh adaptation process is terminated once the maximum amount of cells $\Xi_{max} = 8e6$ is reached.

In addition, we utilize the following parameters. The tolerance for the primal dual active set method is $\varepsilon_2 = 1e-8$, whereas the stopping criteria for the descent method is set to $\varepsilon_{tol} = 1.5e-6$. We tolerate a deviation of $3e-10$ for the determination of the active and biactive sets in Line 7 and 14. The tolerance for solving the primal system (5.146)-(5.147) and the dual systems (5.157) and (5.178) is $1e-15$. Moreover, we use $C_\sigma = 1$ and $\sigma_{max} = 3$. The regularization of the auxiliary problem starts with a penalty parameter $\gamma_0 = 4e6$. The parameter γ is updated (in Line 21) according to the update procedure 4.141 developed in Section 4.3 with a tolerance $tol_c = 1e-3$ for the respective complementarity conditions.

First, we consider the example, where a ring-shaped initial region is trans-

Figure 5.1: The initial state (left), the desired state (middle) and the ansatz functions for the control (right).

formed into a curved channel. The control acts via 16 locally supported ansatz functions, which are evenly distributed over the two-dimensional domain. The ansatz functions along with the initial state and the desired state are depicted in Figure 5.1. For more details on the example we refer to Section 4.3.1, where the example is rigorously introduced.

We depict the evolution of the order parameter φ of the calculated solution in Figure 5.2. It can be seen that the optimal control pushes the upper part of the ring towards the top of the domain whereas the lower part is pushed towards the bottom, which results in a split of the ring-shaped phase into two separate regions at the end of the evolution process. The evolution of the associated slack variable λ is presented in Figure 5.3.

The algorithm terminated after 243 line searches, i.e. Line 27 was executed 243 times. Overall, the mesh was adapted 7 times. In Table 5.1, we list the number of line searches needed for each mesh along with the norm of the final descent direction h_k and the objective value for the calculated solution u_k on the current mesh. We point out that on each mesh we solve entirely different discrete optimization problems, which leads to different optimal objective values.

The primal dual active set method for solving (2.37) terminated after an average of 6 steps. Furthermore, the robustification step, i.e. Line 33, was not needed, since condition (5.180) was satisfied at all times. However, the biactive sets were usually non-empty, which can be seen when comparing the order parameter and the slack variable at the same time instances in Figure 5.2 and Figure 5.3. As a consequence, the algorithm resorted to the penalization method described in Line 19-23 at almost all instances.

Although the results from Algorithm 8 and Algorithm 3 from Section 4.3 are comparable, we point out that the bundle-free method reached the optimal solution after slightly fewer iterations and mesh adaptation steps. Here, we observe that the primal dual active set method leads to a better distinction of the interface and the pure phases. E.g. comparing the final states depicted in Figure 5.2 and Figure 4.9,

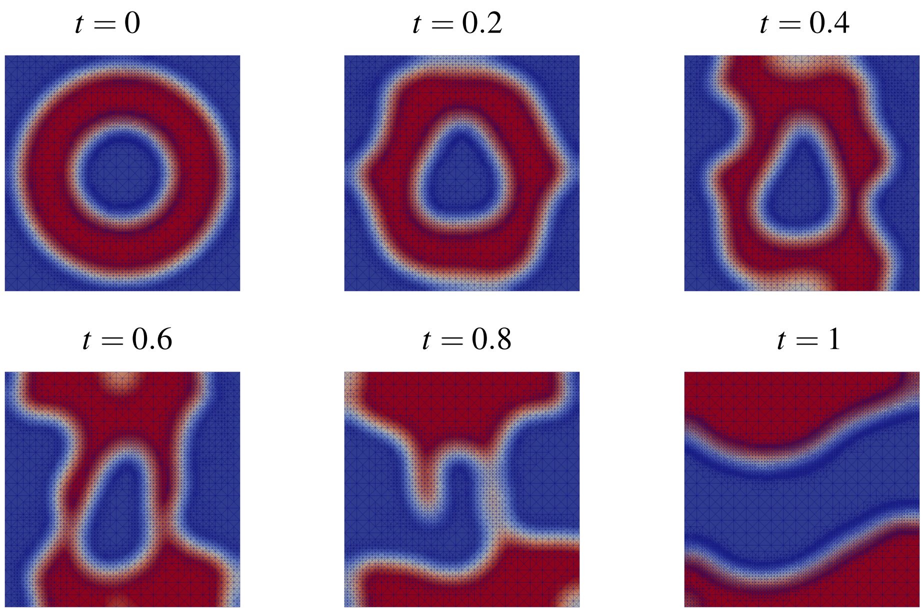

Figure 5.2: The evolution of the phase field over time t.

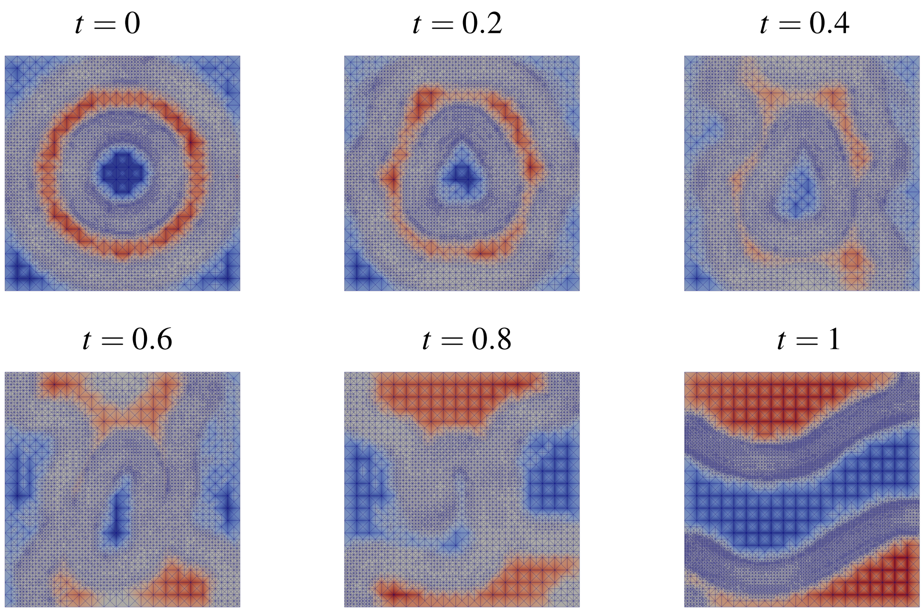

Figure 5.3: The evolution of the associated slack variable a over time t.

Adaptation step	1	2	3	4
Number of cells	1155200	1458074	1890285	2269367
Final objective value	5.03e-03	5.44e-03	5.62e-03	5.09e-03
Norm of final descent direction	7.45e-07	1.02e-06	1.43e-06	8.51e-07
Line searches	139	18	13	28
Adaptation step	5	6	7	Σ
Number of cells	2802236	4076119	5984227	
Final objective value	5.12e-03	4.98e-03	4.95e-03	
Norm of final descent direction	9.18e-07	7.41e-07	7.60e-07	
Line searches	10	16	19	243

Table 5.1: Number of cells, optimal value, norm of the final h_k and number of line searches for each mesh.

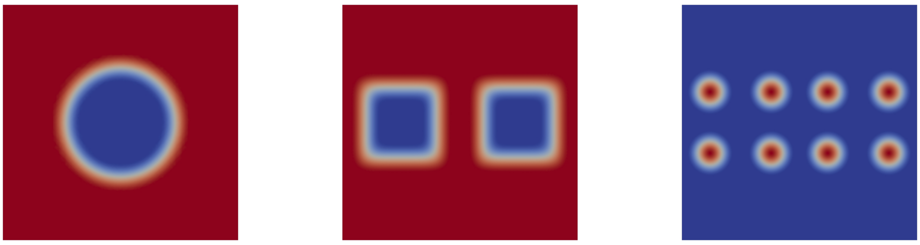

Figure 5.4: The initial state (left), the desired state (middle) and the ansatz functions for the control (right).

it can be seen that the final mesh of the regularization method contains a refined area within the curved channel due to the slowly vanishing presence of the interface. In contrast, the bundle-free implicit programming method managed to reproduce the pure phases of the desired state more precisely.

In the next example, we consider a circular bubble, which is supposed to be split into two square-shaped bubbles under the influence of a gravitational force. The control acts at the corners of each of the two squares, cf. Figure 5.4. For a more precise definition of the example, we refer to Section 4.3.1.

The necessary quantities for the initialization of the algorithm, e.g. the fluid quantities and tolerance parameters, are adopted from the previous example.

In Figure 5.5 the temporal evolution of the order parameter for the computed optimal solution is presented. The calculated optimal objective value for each mesh is shown in Table 5.2. As above, we additionally listed the number of cells, the number of executed line searches, and the norm of the final descent direction associated with each mesh.

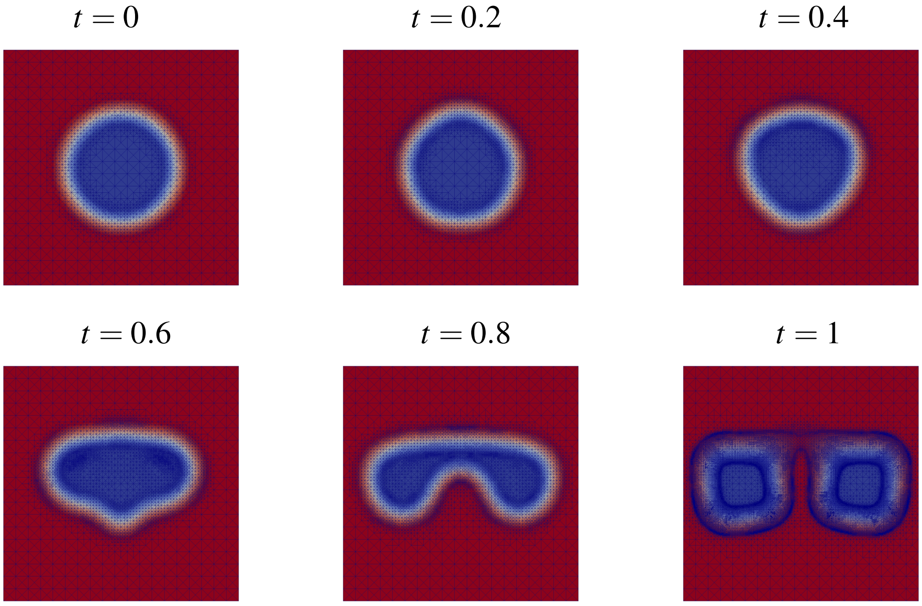

Figure 5.5: The evolution of the phase field over time t.

Adaptation step	1	2	3	4
Number of cells	1155200	1302857	1616325	2183415
Final objective value	4.95e-03	5.74e-03	5.48e-03	5.61e-03
Norm of final descent direction	1.04e-06	1.56e-06	1.61e-06	9.22e-07
Line searches	183	45	27	29

Adaptation step	5	6	7	Σ
Number of cells	2999378	4205147	6050566	
Final objective value	5.10e-03	4.91e-03	4.93e-03	
Norm of final descent direction	8.53e-07	7.19e-07	7.38e-07	
Line searches	39	17	21	361

Table 5.2: Number of cells, optimal value, norm of the final h_k and number of line searches for each mesh.

It can be seen that the algorithm finished considerably faster than the regularization method from Section 4.3. The algorithm terminated after 361 line searches and the mesh adaptation was executed 7 times.

Bibliography

[1] GSL - GNU Scientific Library. `http://www.gnu.org/software/gsl/`

[2] Abels, H.: On a diffuse interface model for two-phase flows of viscous, incompressible fluids with matched densities. Arch. Ration. Mech. Anal. **194**(2), 463–506 (2009)

[3] Abels, H., Breit, D.: Weak solutions for a non-newtonian diffuse interface model with different densities. Nonlinearity **29**(11), 3426 (2016)

[4] Abels, H., Depner, D., Garcke, H.: Existence of weak solutions for a diffuse interface model for two-phase flows of incompressible fluids with different densities. J. Math. Fluid Mech. **15**(3), 453–480 (2013)

[5] Abels, H., Depner, D., Garcke, H.: On an incompressible Navier-Stokes/Cahn-Hilliard system with degenerate mobility. Ann. Inst. H. Poincaré Anal. Non Linéaire **30**(6), 1175–1190 (2013)

[6] Abels, H., Garcke, H., Grün, G.: Thermodynamically consistent, frame indifferent diffuse interface models for incompressible two-phase flows with different densities. Math. Models Methods Appl. Sci. **22**(3), 1150,013, 40 (2012)

[7] Adams, R.A., Fournier, J.J.F.: Sobolev spaces, *Pure and Applied Mathematics (Amsterdam)*, vol. 140, second edn. Elsevier/Academic Press, Amsterdam (2003)

[8] Aland, S.: Time integration for diffuse interface models for two-phase flow. Journal of Computational Physics **262**, 58–71 (2014)

[9] Aland, S., Boden, S., Hahn, A., Klingbeil, F., Weismann, M., Weller, S.: Quantitative comparison of Taylor flow simulations based on sharp-interface and diffuse-interface models. International Journal for Numerical Methods in Fluids **73**(4), 344–361 (2013)

[10] Aland, S., Lowengrub, J., Voigt, A.: Particles at fluid-fluid interfaces: A new Navier-Stokes-Cahn-Hilliard surface-phase-field-crystal model. Physical Review E **86**(4), 046,321 (2012)

[11] Aland, S., Voigt, A.: Benchmark computations of diffuse interface models for two-dimensional bubble dynamics. International Journal for Numerical Methods in Fluids **69**, 747–761 (2012)

[12] Alikakos, N.D., Bates, P.W., Chen, X.: Convergence of the Cahn-Hilliard equation to the Hele-Shaw model. Arch. Rational Mech. Anal. **128**(2), 165–205 (1994)

[13] Amestoy, P., Duff, I., Koster, J., L'Excellent, J.Y.: A fully asynchronous multifrontal solver using distributed dynamic scheduling. SIAM Journal of Matrix Analysis and Applications **23**(1), 15–41 (2001)

[14] Attouch, H.: Variational convergence for functions and operators. Applicable Mathematics Series. Pitman (Advanced Publishing Program), Boston, MA (1984)

[15] Attouch, H., Buttazzo, G., Michaille, G.: Variational analysis in Sobolev and BV spaces: applications to PDEs and optimization. SIAM (2014)

[16] Aubin, J.P.: Applied functional analysis. John Wiley & Sons, New York-Chichester-Brisbane (1979). Translated from the French by Carole Labrousse, With exercises by Bernard Cornet and Jean-Michel Lasry

[17] Balay, S., Abhyankar, S., Adams, M., Brown, J., Brune, P., Buschelman, K., Dalcin, L., Eijkhout, V., Gropp, W., Kaushik, D., Knepley, M., McInnes, L., Rupp, K., Smith, B., Zampini, S., Zhang, H.: PETSc Web page. `http://www.mcs.anl.gov/petsc` (2014)

[18] Barbu, V.: Optimal control of variational inequalities, *Research Notes in Mathematics*, vol. 100. Pitman (Advanced Publishing Program), Boston, MA (1984)

[19] Barbu, V.: Analysis and control of nonlinear infinite-dimensional systems, *Mathematics in Science and Engineering*, vol. 190. Academic Press, Inc., Boston, MA (1993)

[20] Baňas, L., Nürnberg, R.: Adaptive finite element methods for Cahn–Hilliard equations. Journal of Computational and Applied Mathematics **218**, 2–11 (2008)

[21] Bañas, L., Nürnberg, R.: A posteriori estimates for the Cahn–Hilliard equation. Mathematical Modelling and Numerical Analysis **43**(5), 1003–1026 (2009)

[22] Becker, R., Kapp, H., Rannacher, R.: Adaptive finite element methods for optimal control of partial differential equations: basic concept. SIAM J. Control Optim. **39**(1), 113–132 (electronic) (2000)

[23] Becker, R., Kapp, H., Rannacher, R.: Adaptive finite element methods for optimization problems. In: Numerical analysis 1999 (Dundee), *Chapman & Hall/CRC Res. Notes Math.*, vol. 420, pp. 21–42. Chapman & Hall/CRC, Boca Raton, FL (2000)

[24] Bellettini, G., Paolini, M.: Anisotropic motion by mean curvature in the context of Finsler geometry. Hokkaido Math. J. **25**(3), 537–566 (1996)

[25] Benedix, O., Vexler, B.: A posteriori error estimation and adaptivity for elliptic optimal control problems with state constraints. Comput. Optim. Appl. **44**(1), 3–25 (2009)

[26] Bergounioux, M.: Optimal control of an obstacle problem. Appl. Math. Optim. **36**(2), 147–172 (1997)

[27] Bergounioux, M., Dietrich, H.: Optimal control of problems governed by obstacle type variational inequalities: a dual regularization-penalization approach. J. Convex Anal. **5**(2), 329–351 (1998)

[28] Biswas, T., Dharmatti, S., Mohan, M.T.: Maximum principle for some optimal control problems governed by 2D nonlocal Cahn–Hillard–Navier–Stokes equations. Journal of Mathematical Fluid Mechanics **22**, 1–42 (2020)

[29] Blank, L., Butz, M., Garcke, H.: Solving the Cahn–Hilliard variational inequality with a semi-smooth Newton method. ESAIM: Control, Optimisation and Calculus of Variations **17**(4), 931–954 (2011)

[30] Blank, L., Farshbaf-Shaker, M., Garcke, H., Rupprecht, C., Styles, V.: Multi-material phase field approach to structural topology optimization. In: G. Leugering, P. Benner, S. Engell, A. Griewank, H. Harbrecht, M. Hinze, R. Rannacher, S. Ulbrich (eds.) Trends in PDE Constrained Optimization, *International Series of Numerical Mathematics*, vol. 165. Birkhäuser Verlag (2015)

[31] Blowey, J.F., Elliott, C.M.: The Cahn-Hilliard gradient theory for phase separation with nonsmooth free energy. I. Mathematical analysis. European J. Appl. Math. **2**(3), 233–280 (1991)

[32] Boffi, D., Brezzi, F., Fortin, M., et al.: Mixed finite element methods and applications, vol. 44. Springer (2013)

[33] Bogovskiĭ, M.E.: Solution of the first boundary value problem for an equation of continuity of an incompressible medium. Dokl. Akad. Nauk SSSR **248**(5), 1037–1040 (1979)

[34] Bonnans, J.F., Shapiro, A.: Perturbation analysis of optimization problems. Springer, Berlin (2000)

[35] Boyd, S., Boyd, S.P., Vandenberghe, L.: Convex optimization. Cambridge university press (2004)

[36] Boyer, F.: A theoretical and numerical model for the study of incompressible mixture flows. Computers & fluids **31**(1), 41–68 (2002)

[37] Boyer, F., Chupin, L., Fabrie, P.: Numerical study of viscoelastic mixtures through a Cahn-Hilliard flow model. Eur. J. Mech. B Fluids **23**(5), 759–780 (2004)

[38] Boyer, F., Lapuerta, C., Minjeaud, S., Piar, B., Quintard, M.: Cahn–Hilliard/Navier–Stokes model for the simulation of three-phase flows. Transport in Porous Media **82**(3), 463–483 (2010)

[39] Bramble, J., Pasciak, J., Steinbach, O.: On the Stability of the L^2 projection in $H^1(\Omega)$. Mathematics of Computations **71**(237), 147–156 (2001)

[40] Brenner, S.C., Scott, L.R.: The Mathematical Theory of Finite Element Methods, *Texts in Applied Mathematics*, vol. 15. Springer (2008)

[41] Brett, C., Elliott, C.M., Hintermüller, M., Löbhard, C.: Mesh adaptivity in optimal control of elliptic variational inequalities with point-tracking of the state. Interfaces Free Bound. **17**(1), 21–53 (2015)

[42] Brezis, H.: Functional analysis, Sobolev spaces and partial differential equations. Springer Science & Business Media (2010)

[43] Bronsard, L., Kohn, R.V.: Motion by mean curvature as the singular limit of Ginzburg-Landau dynamics. J. Differential Equations **90**(2), 211–237 (1991)

[44] Cahn, J.W., Hilliard, J.E.: Free energy of a nonuniform system. I. Interfacial free energy. The Journal of chemical physics **28**(2), 258–267 (1958)

[45] Chen, X.: Generation and propagation of interfaces for reaction-diffusion equations. J. Differential Equations **96**(1), 116–141 (1992)

[46] Chen, X.: Global asymptotic limit of solutions of the Cahn-Hilliard equation. J. Differential Geom. **44**(2), 262–311 (1996)

[47] Chen, X., Elliott, C.M.: Asymptotics for a parabolic double obstacle problem. Proc. Roy. Soc. London Ser. A **444**(1922), 429–445 (1994)

[48] Clarke, F.H.: A new approach to Lagrange multipliers. Math. Oper. Res. **1**(2), 165–174 (1976)

[49] Cohen, D.S., Murray, J.D.: A generalized diffusion model for growth and dispersal in a population. J. Math. Biol. **12**(2), 237–249 (1981)

[50] Colli, P., Farshbaf-Shaker, M.H., Gilardi, G., Sprekels, J.: Optimal boundary control of a viscous Cahn-Hilliard system with dynamic boundary condition and double obstacle potentials. SIAM J. Control Optim. **53**(4), 2696–2721 (2015)

[51] Colli, P., Gilardi, G., Sprekels, J.: A boundary control problem for the viscous Cahn–Hilliard equation with dynamic boundary conditions. Applied Mathematics & Optimization **73**(2), 195–225 (2016)

[52] Constantin, P., Foias, C.: Navier-Stokes-Equations. The University of Chicago Press (1988)

[53] Copetti, M.I.M., Elliott, C.M.: Kinetics of phase decomposition processes: numerical solutions to Cahn–Hilliard equation. Materials Science and Technology **6**(3), 273–284 (1990)

[54] De Giorgi, E.: Sulla convergenza di alcune successioni d'integrali del tipo dell'area. Rend. Mat. (6) **8**, 277–294 (1975). Collection of articles dedicated to Mauro Picone on the occasion of his ninetieth birthday

[55] De Giorgi, E., Franzoni, T.: Su un tipo di convergenza variazionale. Atti Accad. Naz. Lincei Rend. Cl. Sci. Fis. Mat. Natur. (8) **58**(6), 842–850 (1975)

[56] De Mottoni, P., Schatzman, M.: Geometrical evolution of developed interfaces. Transactions of the American Mathematical Society **347**(5), 1533–1589 (1995)

[57] Deckelnick, K., Günther, A., Hinze, M.: Finite element approximation of elliptic control problems with constraints on the gradient. Numer. Math. **111**(3), 335–350 (2009)

[58] Deckelnick, K., Hinze, M.: Semidiscretization and error estimates for distributed control of the instationary Navier-Stokes equations. Numerische Mathematik **97**(2), 297–320 (2004)

[59] Delfour, M.C., Zolésio, J.P.: Shapes and geometries: Analysis. Differential Calculus, and Optimization, SIAM, Philadelphia p. 482 (2001)

[60] Ding, H., Spelt, P.D., Shu, C.: Diffuse interface model for incompressible two-phase flows with large density ratios. Journal of Computational Physics **226**(2), 2078–2095 (2007)

[61] Dörfler, W.: A convergent adaptive algorithm for Poisson's equation. SIAM Journal on Numerical Analysis **33**(3), 1106–1124 (1996)

[62] Eckert, S., Nikrityuk, P.A., Willers, B., Räbiger, D., Shevchenko, N., Neumann-Heyme, H., Travnikov, V., Odenbach, S., Voigt, A., Eckert, K.: Electromagnetic melt flow control during solidification of metallic alloys. The European Physical Journal Special Topics **220**(1), 123–137 (2013)

[63] Ekeland, I., Témam, R.: Convex analysis and variational problems, *Classics in Applied Mathematics*, vol. 28, english edn. Society for Industrial and Applied Mathematics (SIAM), Philadelphia, PA (1999). Translated from the French

[64] Elliott, C., Stinner, B., Styles, V., Welford, R.: Numerical computation of advection and diffusion on evolving diffuse interfaces. IMA Journal of Numerical Analysis **31**(3), 786–812 (2011)

[65] Elliott, C.M., French, D.A., Milner, F.: A second order splitting method for the cahn-hilliard equation. Numerische Mathematik **54**(5), 575–590 (1989)

[66] Elliott, C.M., Garcke, H.: On the Cahn-Hilliard equation with degenerate mobility. SIAM J. Math. Anal. **27**(2), 404–423 (1996)

[67] Elliott, C.M., Larsson, S.: Error estimates with smooth and nonsmooth data for a finite element method for the Cahn–Hilliard equation. Mathematics of Computation **58**(198), 603–630 (1992)

[68] Elliott, C.M., Songmu, Z.: On the Cahn-Hilliard equation. Arch. Rational Mech. Anal. **96**(4), 339–357 (1986)

[69] Evans, L.C., Soner, H.M., Souganidis, P.E.: Phase transitions and generalized motion by mean curvature. Comm. Pure Appl. Math. **45**(9), 1097–1123 (1992)

[70] Facchinei, F., Jiang, H., Qi, L.: A smoothing method for mathematical programs with equilibrium constraints. Math. Program. **85**(1, Ser. A), 107–134 (1999)

[71] Fife, P.C.: Models for phase separation and their mathematics. Electron. J. Differential Equations (48), 1–26 (2000)

[72] Fletcher, R., Leyffer, S., Ralph, D., Scholtes, S.: Local convergence of SQP methods for mathematical programs with equilibrium constraints. SIAM J. Optim. **17**(1), 259–286 (2006)

[73] Friedman, A.: Optimal control for variational inequalities. SIAM J. Control Optim. **24**(3), 439–451 (1986)

[74] Frigeri, S., Gal, C.G., Grasselli, M.: On Nonlocal Cahn–Hilliard–Navier–Stokes Systems in Two Dimensions. Journal of Nonlinear Science **26**(4), 847–893 (2016)

[75] Frigeri, S., Gal, C.G., Grasselli, M., Sprekels, J.: Two-dimensional nonlocal Cahn-Hilliard-Navier-Stokes systems with variable viscosity, degenerate mobility and singular potential. Nonlinearity **32**(2), 678–727 (2019)

[76] Frigeri, S., Rocca, E., Sprekels, J.: Optimal distributed control of a nonlocal Cahn-Hilliard/Navier-Stokes system in two dimensions. SIAM J. Control Optim. **54**(1), 221–250 (2016)

[77] Gal, C.G., Grasselli, M.: Asymptotic behavior of a Cahn-Hilliard-Navier-Stokes system in 2D. Ann. Inst. H. Poincaré Anal. Non Linéaire **27**(1), 401–436 (2010)

[78] Galdi, G.P.: An introduction to the mathematical theory of the Navier-Stokes equations. Vol. I, *Springer Tracts in Natural Philosophy*, vol. 38. Springer-Verlag, New York (1994). Linearized steady problems

[79] Garcia, C.E., Prett, D.M., Morari, M.: Model predictive control: Theory and practice – a survey. Automatica **25**(3), 335–348 (1989)

[80] Garcke, H., Hecht, C., Hinze, M., Kahle, C.: Numerical approximation of phase field based shape and topology optimization for fluids. SIAM Journal on Scientific Computing **37**(4), 1846–1871 (2015)

[81] Garcke, H., Hinze, M., Kahle, C.: A stable and linear time discretization for a thermodynamically consistent model for two-phase incompressible flow. Applied Numerical Mathematics **99**, 151 – 171 (2016)

[82] Garcke, H., Hinze, M., Kahle, C.: Optimal control of time-discrete two-phase flow driven by a diffuse-interface model. ESAIM: Control, Optimisation and Calculus of Variations **25**, 13 (2019)

[83] Garcke, H., Lam, K.F., Stinner, B.: Diffuse interface modelling of soluble surfactants in two-phase flow. Communications in Mathematical Sciences **12**(8), 1475–1522 (2014)

[84] Girault, V., Raviart, P.A.: Finite element methods for Navier-Stokes equations, *Springer Series in Computational Mathematics*, vol. 5. Springer-Verlag, Berlin (1986). Theory and algorithms

[85] Glowinski, R., Lions, J.L., Trémolières, R.: Numerical analysis of variational inequalities, *Studies in Mathematics and its Applications*, vol. 8. North-Holland Publishing Co., Amsterdam-New York (1981). Translated from the French

[86] Goldberg, H., Kampowsky, W., Tröltzsch, F.: On Nemytskij operators in L_p-spaces of abstract functions. Math. Nachr. **155**, 127–140 (1992)

[87] Grün, G.: On convergent schemes for diffuse interface models for two-phase flow of incompressible fluids with general mass densities. SIAM Journal on Numerical Analysis **51**(6), 3036–3061 (2013)

[88] Grün, G., Guillén-Gonzáles, F., Metzger, S.: On Fully Decoupled Convergent Schemes for Diffuse Interface Models for Two-Phase Flow with General Mass Densities. Communications in Computational Physics **19**(5), 1473–1502 (2016)

[89] Grün, G., Klingbeil, F.: Two-phase flow with mass density contrast: Stable schemes for a thermodynamic consistent and frame indifferent diffuse interface model. Journal of Computational Physics **257**(A), 708–725 (2014)

[90] Guillén-Gonzáles, F., Tierra, G.: Splitting schemes for a Navier–Stokes–Cahn–Hilliard model for two fluids with different densities. Journal of Computational Mathematics **32**(6), 643–664 (2014)

[91] Günther, A., Hinze, M.: A posteriori error control of a state constrained elliptic control problem. J. Numer. Math. **16**(4), 307–322 (2008)

[92] Günther, A., Hinze, M.: Elliptic control problems with gradient constraints—variational discrete versus piecewise constant controls. Comput. Optim. Appl. **49**(3), 549–566 (2011)

[93] Guo, Z., Lin, P., Lowengrub, J.S.: A numerical method for the quasi-incompressible Cahn–Hilliard–Navier–Stokes equations for variable density flows with a discrete energy law. Journal of Computational Physics **276**, 486–507 (2014)

[94] Gurtin, M.E., Polignone, D., Viñals, J.: Two-phase binary fluids and immiscible fluids described by an order parameter. Math. Models Methods Appl. Sci. **6**(6), 815–831 (1996)

[95] Henrot, A., Pierre, M.: Variation et optimisation de formes, volume 48 of Mathématiques & Applications (Berlin)[Mathematics & Applications]. Springer, Berlin (2005)

[96] Héron, B.: Quelques propriétés des applications de trace dans des espaces de champs de vecteurs à divergence nulle. Comm. Partial Differential Equations **6**(12), 1301–1334 (1981)

[97] Herzog, R., Meyer, C., Wachsmuth, G.: C-stationarity for optimal control of static plasticity with linear kinematic hardening. SIAM J. Control Optim. **50**(5), 3052–3082 (2012)

[98] Herzog, R., Meyer, C., Wachsmuth, G.: B- and strong stationarity for optimal control of static plasticity with hardening. SIAM J. Optim. **23**(1), 321–352 (2013)

[99] Hintermüller, M.: Semismooth newton methods and applications. Department of Mathematics, Humboldt-University of Berlin (2010)

[100] Hintermüller, M., Hinze, M., Hoppe, R.H.: Weak-duality based adaptive finite element methods for pde-constrained optimization with pointwise gradient state-constraints. J. Comput. Math **30**(2), 101–123 (2012)

[101] Hintermüller, M., Hinze, M., Kahle, C.: An adaptive finite element Moreau–Yosida-based solver for a coupled Cahn–Hilliard/Navier–Stokes system. Journal of Computational Physics **235**, 810–827 (2013)

[102] Hintermüller, M., Hinze, M., Kahle, C., Keil, T.: A goal-oriented dual-weighted adaptive finite element approach for the optimal control of a nonsmooth Cahn-Hilliard-Navier-Stokes system. Optim. Eng. **19**(3), 629–662 (2018)

[103] Hintermüller, M., Hinze, M., Tber, M.H.: An adaptive finite-element Moreau-Yosida-based solver for a non-smooth Cahn-Hilliard problem. Optim. Methods Softw. **26**(4-5), 777–811 (2011)

[104] Hintermüller, M., Hoppe, R.H.: Adaptive finite element methods for control constrained distributed and boundary optimal control problems. Numerical PDE Constrained Optimization **73** (2008)

[105] Hintermüller, M., Hoppe, R.H., Iliash, Y., Kieweg, M.: An a posteriori error analysis of adaptive finite element methods for distributed elliptic control problems with control constraints. ESAIM: Control, Optimisation and Calculus of Variations **14**(3), 540–560 (2008)

[106] Hintermüller, M., Hoppe, R.H.W.: Goal-oriented adaptivity in control constrained optimal control of partial differential equations. SIAM J. Control Optim. **47**(4), 1721–1743 (2008)

[107] Hintermüller, M., Hoppe, R.H.W.: Goal-oriented adaptivity in pointwise state constrained optimal control of partial differential equations. SIAM J. Control Optim. **48**(8), 5468–5487 (2010)

[108] Hintermüller, M., Hoppe, R.H.W., Löbhard, C.: Dual-weighted goal-oriented adaptive finite elements for optimal control of elliptic variational inequalities. ESAIM Control Optim. Calc. Var. **20**(2), 524–546 (2014)

[109] Hintermüller, M., Ito, K., Kunisch, K.: The primal-dual active set strategy as a semismooth Newton method. SIAM J. Optim. **13**(3), 865–888 (2003) (2002)

[110] Hintermüller, M., Keil, T., Wegner, D.: Optimal control of a semidiscrete Cahn-Hilliard-Navier-Stokes system with nonmatched fluid densities. SIAM J. Control Optim. **55**(3), 1954–1989 (2017)

[111] Hintermüller, M., Kopacka, I.: Mathematical programs with complementarity constraints in function space: *C*- and strong stationarity and a path-following algorithm. SIAM J. Optim. **20**(2), 868–902 (2009)

[112] Hintermüller, M., Kopacka, I.: A smooth penalty approach and a nonlinear multigrid algorithm for elliptic MPECs. Computational Optimization and Applications **50**(1), 111–145 (2011)

[113] Hintermüller, M., Mordukhovich, B.S., Surowiec, T.M.: Several approaches for the derivation of stationarity conditions for elliptic MPECs with upper-level control constraints. Math. Program. **146**(1-2, Ser. A), 555–582 (2014)

[114] Hintermüller, M., Schiela, A., Wollner, W.: The length of the primal-dual path in Moreau-Yosida-based path-following methods for state constrained optimal control. SIAM J. Optim. **24**(1), 108–126 (2014)

[115] Hintermüller, M., Surowiec, T.: A bundle-free implicit programming approach for a class of elliptic MPECs in function space. Mathematical Programming **160**(1), 271–305 (2016)

[116] Hintermüller, M., Ulbrich, M.: A mesh-independence result for semismooth Newton methods. Math. Program. **101**(1, Ser. B), 151–184 (2004)

[117] Hintermüller, M., Wegner, D.: Distributed optimal control of the Cahn-Hilliard system including the case of a double-obstacle homogeneous free energy density. SIAM J. Control Optim. **50**(1), 388–418 (2012)

[118] Hintermüller, M., Wegner, D.: Optimal control of a semidiscrete Cahn-Hilliard-Navier-Stokes system. SIAM J. Control Optim. **52**(1), 747–772 (2014)

[119] Hinze, M.: Optimal and instantaneous control of the instationary Navier-Stokes equations (1999). Habilitationsschrift

[120] Hinze, M.: Instantaneous closed loop control of the Navier–Stokes system. SIAM Journal on Control and Optimization **44**(2), 564–583 (2005)

[121] Hinze, M., Kahle, C.: A nonlinear Model Predictive Concept for the Control of Two-Phase Flows governed by the Cahn–Hilliard Navier–Stokes System. In: System Modeling and Optimization, vol. 391 in IFIP Advances in Information and Communication Technology (2013)

[122] Hinze, M., Kunisch, K.: On suboptimal control strategies for the navier-stokes equations. In: ESAIM: Proceedings, vol. 4, pp. 181–198. EDP Sciences (1998)

[123] Hohenberg, P.C., Halperin, B.I.: Theory of dynamic critical phenomena. Reviews of Modern Physics **49**(3), 435 (1977)

[124] Hysing, S., Turek, S., Kuzmin, D., Parolini, N., Burman, E., Ganesan, S., Tobiska, L.: Quantitative benchmark computations of two-dimensional bubble dynamics. International Journal for Numerical Methods in Fluids **60**(11), 1259–1288 (2009)

[125] Ito, K., Kunisch, K.: Optimal control of elliptic variational inequalities. Appl. Math. Optim. **41**(3), 343–364 (2000)

[126] Ito, K., Kunisch, K.: Semi–smooth newton methods for variational inequalities of the first kind. ESAIM: Mathematical Modelling and Numerical Analysis **37**(1), 41–62 (2003)

[127] Jarušek, J., Krbec, M., Rao, M., Sokołowski, J.: Conical differentiability for evolution variational inequalities. J. Differential Equations **193**(1), 131–146 (2003)

[128] John, V., Linke, A., Merdon, C., Neilan, M., Rebholz, L.G.: On the divergence constraint in mixed finite element methods for incompressible flows. SIAM Rev. **59**(3), 492–544 (2017)

[129] Kahle, C.: A L^∞ bound for the Cahn–Hilliard equation with relaxed non-smooth free energy density. arXiv:1511.02618 (2015)

[130] Kay, D., Styles, V., Welford, R.: Finite element approximation of a Cahn–Hilliard–Navier–Stokes system. Interfaces and Free Boundaries **10**(1), 15–43 (2008)

[131] Kim, J., Kang, K., Lowengrub, J.: Conservative multigrid methods for Cahn-Hilliard fluids. J. Comput. Phys. **193**(2), 511–543 (2004)

[132] Kim, J., Lowengrub, J.: Interfaces and multicomponent fluids. Encyclopedia of Mathematical Physics pp. 135–144 (2004)

[133] Kinderlehrer, D., Stampacchia, G.: An introduction to variational inequalities and their applications, *Classics in Applied Mathematics*, vol. 31. Society for Industrial and Applied Mathematics (SIAM), Philadelphia, PA (2000). Reprint of the 1980 original

[134] Kopacka, I.: MPECs/MPCCs in function space: first order optimality concepts, path-following, and multilevel algorithms. Ph.D. thesis, Karl-Franzens-Universität Graz (2009)

[135] Layton, W.: Introduction to the numerical analysis of incompressible viscous flows. SIAM (2008)

[136] Linke, A., Merdon, C.: Pressure-robustness and discrete Helmholtz projectors in mixed finite element methods for the incompressible Navier–Stokes equations. Computer Methods in Applied Mechanics and Engineering **311**, 304–326 (2016)

[137] Lions, J.: Various topics in the theory of optimal control of distributed systems. In: Optimal Control Theory and its Applications, pp. 166–309. Springer (1974)

[138] Lions, J., Magenes, E.: Non-Homogeneous Boundary Value Problems and Applications. Springer Verlag Berlin Heidelberg (1972)

[139] Lions, J.L., Stampacchia, G.: Variational inequalities. Communications on pure and applied mathematics **20**(3), 493–519 (1967)

[140] Logg, A., Mardal, K.A., Wells, G. (eds.): Automated Solution of Differential Equations by the Finite Element Method - The FEniCS Book, *Lecture Notes in Computational Science and Engineering*, vol. 84. Springer (2012)

[141] Lowengrub, J., Truskinovsky, L.: Quasi-incompressible Cahn-Hilliard fluids and topological transitions. R. Soc. Lond. Proc. Ser. A Math. Phys. Eng. Sci. **454**(1978), 2617–2654 (1998)

[142] Luo, Z.Q., Pang, J.S., Ralph, D.: Mathematical programs with equilibrium constraints. Cambridge University Press, Cambridge (1996)

[143] Luo, Z.Q., Pang, J.S., Ralph, D., Wu, S.Q.: Exact penalization and stationarity conditions of mathematical programs with equilibrium constraints. Math. Programming **75**(1, Ser. A), 19–76 (1996)

[144] Maugeri, A., Palagachev, D.K., Softova, L.G.: Elliptic and parabolic equations with discontinuous coefficients, *Mathematical Research*, vol. 109. Wiley-VCH Verlag Berlin GmbH, Berlin (2000)

[145] Maz'ya, V.: Sobolev spaces. Springer (2013)

[146] Medjo, T.: Optimal control of a Cahn-Hilliard-Navier-Stokes model with state constraints. J. Convex Anal. **22**(4), 1135–1172 (2015)

[147] Meyer, C., Rademacher, A., Wollner, W.: Adaptive optimal control of the obstacle problem. SIAM J. Sci. Comput. **37**(2), A918–A945 (2015)

[148] Mignot, F.: Contrôle dans les inéquations variationelles elliptiques. J. Functional Analysis **22**(2), 130–185 (1976)

[149] Mignot, F., Puel, J.P.: Optimal control in some variational inequalities. SIAM J. Control Optim. **22**(3), 466–476 (1984)

[150] Modica, L.: The gradient theory of phase transitions and the minimal interface criterion. Arch. Rational Mech. Anal. **98**(2), 123–142 (1987)

[151] Mordukhovich, B.S.: Variational analysis and generalized differentiation. I, *Grundlehren der Mathematischen Wissenschaften [Fundamental Principles of Mathematical Sciences]*, vol. 330. Springer-Verlag, Berlin (2006). Basic theory

[152] Mordukhovich, B.S.: Variational analysis and generalized differentiation. II, *Grundlehren der Mathematischen Wissenschaften [Fundamental Principles of Mathematical Sciences]*, vol. 331. Springer-Verlag, Berlin (2006). Applications

[153] Nochetto, R.H., Paolini, M., Verdi, C.: Optimal interface error estimates for the mean curvature flow. Ann. Scuola Norm. Sup. Pisa Cl. Sci. (4) **21**(2), 193–212 (1994)

[154] Nochetto, R.H., Siebert, K.G., Veeser, A.: Pointwise a posteriori error control for elliptic obstacle problems. Numer. Math. **95**(1), 163–195 (2003)

[155] Nochetto, R.H., Verdi, C.: Combined effect of explicit time-stepping and quadrature for curvature driven flows. Numer. Math. **74**(1), 105–136 (1996)

[156] Novick-Cohen, A., Segel, L.A.: Nonlinear aspects of the Cahn-Hilliard equation. Phys. D **10**(3), 277–298 (1984)

[157] Oono, Y., Puri, S.: Study of phase-separation dynamics by use of cell dynamical systems. I. Modeling. Physical Review A **38**(1), 434–463 (1988)

[158] Oono, Y., Puri, S.: Study of phase-separation dynamics by use of cell dynamical systems. II. Two-dimensional demonstrations. Physical Review A **38**(3), 1542 (1988)

[159] Outrata, J., Jarušek, J., Stará, J.: On optimality conditions in control of elliptic variational inequalities. Set-Valued Var. Anal. **19**(1), 23–42 (2011)

[160] Outrata, J., Kočvara, M., Zowe, J.: Nonsmooth approach to optimization problems with equilibrium constraints: theory, applications and numerical results, *Nonconvex Optimization and its Applications*, vol. 28. Kluwer Academic Publishers, Dordrecht (1998)

[161] Pego, R.L.: Front migration in the nonlinear Cahn-Hilliard equation. Proc. Roy. Soc. London Ser. A **422**(1863), 261–278 (1989)

[162] Praetorius, S., Voigt, A.: A navier-stokes phase-field crystal model for colloidal suspensions. The Journal of chemical physics **142**(15) (2015)

[163] Prüss, J., Racke, R., Zheng, S.: Maximal regularity and asymptotic behavior of solutions for the Cahn-Hilliard equation with dynamic boundary conditions. Ann. Mat. Pura Appl. (4) **185**(4), 627–648 (2006)

[164] Qi, L., Sun, J.: A nonsmooth version of Newton's method. Mathematical programming **58**(1), 353–367 (1993)

[165] Rockafellar, R.T.: On the maximal monotonicity of subdifferential mappings. Pacific J. Math. **33**, 209–216 (1970)

[166] Rubinstein, J., Sternberg, P., Keller, J.B.: Fast reaction, slow diffusion, and curve shortening. SIAM J. Appl. Math. **49**(1), 116–133 (1989)

[167] Ruszczyński, A.: Nonlinear optimization. Princeton University Press, Princeton, NJ (2006)

[168] Scheel, H.: Ein Straffunktionsansatz für Optimierungsprobleme mit Gleichgewichtsrestriktionen. Master's thesis, Universität Karlsruhe, Institut für Stochastik und mathematische Wirtschaftstheorie, 76128 Karlsruhe (1995)

[169] Scheel, H., Scholtes, S.: Mathematical programs with complementarity constraints: stationarity, optimality, and sensitivity. Math. Oper. Res. **25**(1), 1–22 (2000)

[170] Schiela, A., Wachsmuth, D.: Convergence analysis of smoothing methods for optimal control of stationary variational inequalities with control constraints. ESAIM Math. Model. Numer. Anal. **47**(3), 771–787 (2013)

[171] Schmidt, A., Siebert, K.G.: Design of adaptive finite element software: The finite element toolbox ALBERTA, *Lecture Notes in Computational Science and Engineering*, vol. 42. Springer (2005)

[172] Scholtes, S.: Convergence properties of a regularization scheme for mathematical programs with complementarity constraints. SIAM J. Optim. **11**(4), 918–936 (2001)

[173] Shapiro, A.: On concepts of directional differentiability. J. Optim. Theory Appl. **66**(3), 477–487 (1990)

[174] Shen, J., Yang, X.: A Phase-Field Model and its Numerical Approximation for Two-Phase Incompressible Flows with Different Densities and Viscosities. SIAM Journal on Scientific Computing **32**(3), 1159–1179 (2010)

[175] Showalter, R.E.: Monotone operators in Banach space and nonlinear partial differential equations, *Mathematical Surveys and Monographs*, vol. 49. American Mathematical Society, Providence, RI (1997)

[176] Smolders, C., Van Aartsen, J., Steenbergen, A.: Liquid-liquid phase separation in concentrated solutions of non-crystallizable polymers by spinodal decomposition. Kolloid-Zeitschrift und Zeitschrift für Polymere **243**(1), 14–20 (1971)

[177] Stauffer, D.: Application of the generalized landau ansatz to second order phase transitions. Zeitschrift für Physik A Hadrons and nuclei **221**(2), 122–133 (1969)

[178] Stoth, B.E.E.: Convergence of the Cahn-Hilliard equation to the Mullins-Sekerka problem in spherical symmetry. J. Differential Equations **125**(1), 154–183 (1996)

[179] Tayler, A.B.: Mathematical models in applied mechanics. Oxford Applied Mathematics and Computing Science Series. The Clarendon Press, Oxford University Press, New York (1986)

[180] Temam, R.: Navier-Stokes equations. Theory and numerical analysis. North-Holland Publishing Co., Amsterdam-New York-Oxford (1977). Studies in Mathematics and its Applications, Vol. 2

[181] Tiba, D.: Optimal control of nonsmooth distributed parameter systems, *Lecture Notes in Mathematics*, vol. 1459. Springer-Verlag, Berlin (1990)

[182] Tröltzsch, F.: Optimal control of partial differential equations: theory, methods and applications, *Graduate Studies in Mathematics*, vol. 112. American Mathematical Society, Providence, RI (2010). Translated from the 2005 German original by Jürgen Sprekels

[183] Tsutsumi, M., Yasuda, T.: Penalty method for variational inequalities and its error estimates. Funkcialaj Ekvacioj Serio Internacia **42**, 281–290 (1999)

[184] Verfürth, R.: A posteriori error analysis of space-time finite element discretizations of the time-dependent Stokes equations. Calcolo **47**(3), 149–167 (2010)

[185] Vexler, B., Wollner, W.: Adaptive finite elements for elliptic optimization problems with control constraints. SIAM J. Control Optim. **47**(1), 509–534 (2008)

[186] Wachsmuth, G.: Towards M-stationarity for optimal control of the obstacle problem with control constraints. SIAM J. Control Optim. **54**(2), 964–986 (2016)

[187] Wang, Q.F., Nakagiri, S.I.: Weak solutions of Cahn-Hilliard equations having forcing terms and optimal control problems. Sūrikaisekikenkyūsho Kōkyūroku (1128), 172–180 (2000). Mathematical models in functional equations (Japanese) (Kyoto, 1999)

[188] Ye, J.J.: Necessary and sufficient optimality conditions for mathematical programs with equilibrium constraints. J. Math. Anal. Appl. **307**(1), 350–369 (2005)

[189] Yong, J.M., Zheng, S.M.: Feedback stabilization and optimal control for the Cahn-Hilliard equation. Nonlinear Anal. **17**(5), 431–444 (1991)

[190] Zhou, B., et al.: Simulations of polymeric membrane formation in 2D and 3D. Ph.D. thesis, Massachusetts Institute of Technology (2006)

[191] Zowe, J., Kurcyusz, S.: Regularity and stability for the mathematical programming problem in Banach spaces. Appl. Math. Optim. **5**(1), 49–62 (1979)